



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 03:35 PM EDT

PDB ID : 3F8U  
Title : Tapasin/ERp57 heterodimer  
Authors : Dong, G.; Reinisch, K.M.  
Deposited on : 2008-11-13  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

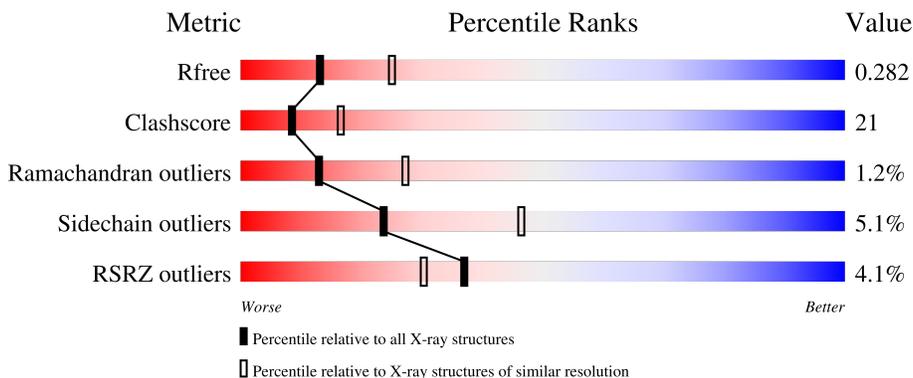
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	 69% 25% . .
1	C	481	 62% 30% . .
2	B	401	 59% 27% . 10%
2	D	401	 58% 29% . 10%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13051 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein disulfide-isomerase A3ERp57.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	3724	2362	625	724	13	0	0	0
1	C	462	3675	2335	617	710	13	0	0	0

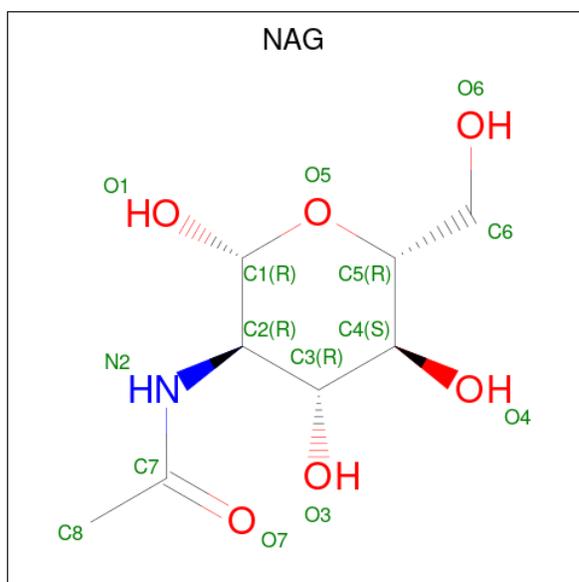
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ALA	CYS	engineered mutation	UNP P30101
C	60	ALA	CYS	engineered mutation	UNP P30101

- Molecule 2 is a protein called Tapasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	361	2755	1766	486	492	11	0	0	0
2	D	361	2757	1769	486	491	11	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	B	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	36	36	36	0	0
4	B	49	49	49	0	0
4	C	7	7	7	0	0
4	D	20	20	20	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.10Å 72.30Å 200.19Å 90.00° 94.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 49.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.60) 94.8 (49.89-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.245 , 0.285 0.247 , 0.282	Depositor DCC
$R_{free}$ test set	3296 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtrriage
Anisotropy	0.151	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.42	0/3808	0.63	0/5142
1	C	0.36	0/3758	0.60	0/5073
2	B	0.40	0/2849	0.70	4/3906 (0.1%)
2	D	0.38	0/2849	0.70	2/3905 (0.1%)
All	All	0.39	0/13264	0.65	6/18026 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	ASP	N-CA-C	5.82	126.70	111.00
2	B	41	ASP	N-CA-C	5.63	126.21	111.00
2	B	342	LEU	CA-CB-CG	5.58	128.12	115.30
2	D	342	LEU	CA-CB-CG	5.50	127.94	115.30
2	B	255	LEU	CA-CB-CG	-5.48	102.69	115.30
2	B	196	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3724	0	3619	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3675	0	3578	186	0
2	B	2755	0	2713	111	0
2	D	2757	0	2720	107	0
3	B	14	0	13	0	0
3	D	14	0	13	1	0
4	A	36	0	0	1	0
4	B	49	0	0	2	0
4	C	7	0	0	0	0
4	D	20	0	0	1	0
All	All	13051	0	12656	532	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG21	1:A:47:LEU:N	1.70	1.06
1:C:215:PHE:CE1	1:C:285:MET:HA	1.92	1.05
2:B:317:GLY:O	2:B:321:GLN:CG	2.08	1.01
2:D:283:ARG:HA	2:D:381:GLU:HB3	1.43	1.00
1:A:448:ARG:HG3	1:A:449:GLY:H	1.26	0.98
1:C:448:ARG:HG3	1:C:449:GLY:H	1.27	0.97
2:D:42:PRO:HG3	2:D:131:LEU:HG	1.47	0.96
2:B:317:GLY:O	2:B:321:GLN:HG3	1.65	0.96
2:B:132:ILE:HD13	2:B:133:THR:N	1.81	0.95
2:B:42:PRO:HG3	2:B:131:LEU:HG	1.44	0.95
1:A:308:SER:HA	1:A:311:LEU:HD23	1.46	0.95
2:B:283:ARG:HA	2:B:381:GLU:HB3	1.46	0.95
1:A:32:ASP:H	1:A:88:ASN:HD22	1.07	0.94
1:C:32:ASP:H	1:C:88:ASN:HD22	1.01	0.93
1:C:308:SER:HA	1:C:311:LEU:HD23	1.51	0.93
1:C:130:LYS:HZ1	1:C:184:PHE:H	1.15	0.92
2:D:160:LEU:H	2:D:235:THR:HG22	1.34	0.91
2:B:160:LEU:H	2:B:235:THR:HG22	1.36	0.90
1:C:142:GLU:HG2	1:C:192:LEU:HD21	1.56	0.88
1:A:142:GLU:HG2	1:A:192:LEU:HD21	1.56	0.87
1:C:100:TYR:OH	2:D:97:ARG:HG3	1.74	0.87
2:B:233:ASN:OD1	2:B:235:THR:HG23	1.75	0.87
2:D:233:ASN:OD1	2:D:235:THR:HG23	1.75	0.87
1:C:323:ILE:HD12	1:C:323:ILE:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ILE:HG13	1:C:244:CYS:N	1.91	0.84
1:C:32:ASP:H	1:C:88:ASN:ND2	1.73	0.84
1:A:32:ASP:H	1:A:88:ASN:ND2	1.76	0.84
2:B:60:ARG:HA	2:B:60:ARG:HH11	1.43	0.84
1:A:203:ILE:HD12	1:A:232:ILE:HD12	1.59	0.84
2:D:34:PRO:O	2:D:130:VAL:HG21	1.78	0.83
2:D:60:ARG:HA	2:D:60:ARG:HH11	1.44	0.81
1:C:426:ASP:OD1	1:C:429:ILE:HD13	1.80	0.81
2:B:317:GLY:O	2:B:321:GLN:HG2	1.81	0.80
2:B:90:THR:HG22	2:B:90:THR:O	1.81	0.79
1:C:130:LYS:NZ	1:C:184:PHE:H	1.80	0.79
1:C:119:ARG:HH11	1:C:119:ARG:HG2	1.50	0.77
1:A:323:ILE:HD12	1:A:323:ILE:H	1.49	0.76
1:A:222:TYR:CE2	1:A:232:ILE:HD13	2.21	0.76
2:B:59:PHE:HZ	2:B:108:ILE:HG21	1.49	0.76
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.51	0.75
1:C:477:ILE:HG23	1:C:490:ILE:HD13	1.68	0.75
2:B:47:SER:N	2:B:132:ILE:HD11	2.02	0.74
1:A:367:SER:HB2	1:A:383:ALA:HB3	1.68	0.74
2:D:90:THR:HG22	2:D:90:THR:O	1.87	0.74
2:B:79:LEU:HD12	2:B:80:PRO:HD2	1.68	0.74
1:C:215:PHE:HE1	1:C:285:MET:HA	1.51	0.74
2:D:160:LEU:HD21	2:D:253:ILE:HD11	1.69	0.74
2:B:47:SER:HB2	2:B:132:ILE:HD12	1.71	0.73
2:D:34:PRO:HG2	2:D:130:VAL:CG2	2.19	0.72
1:C:367:SER:HB2	1:C:383:ALA:HB3	1.70	0.72
1:C:64:ALA:HB3	1:C:65:PRO:HD3	1.71	0.72
1:A:93:ASN:ND2	2:B:97:ARG:HH12	1.88	0.71
1:A:77:ILE:HG22	1:A:78:VAL:HG23	1.72	0.71
1:A:382:VAL:H	1:A:385:ASN:HD21	1.37	0.71
1:C:133:GLY:N	1:C:179:ARG:HH12	1.88	0.71
1:A:42:THR:HG22	1:A:43:GLY:N	2.05	0.70
1:C:31:THR:HB	1:C:88:ASN:HD21	1.55	0.70
2:D:52:ALA:HB1	2:D:163:ALA:HB1	1.73	0.70
1:C:399:ILE:HD13	1:C:400:GLU:N	2.06	0.69
1:C:130:LYS:HE2	1:C:182:TYR:O	1.91	0.69
1:A:260:LEU:HD21	1:A:262:ILE:HD11	1.73	0.69
1:A:93:ASN:HD22	2:B:97:ARG:HH12	1.40	0.69
1:A:425:LYS:HE3	1:A:491:GLN:HE21	1.56	0.69
1:C:448:ARG:HG3	1:C:449:GLY:N	2.07	0.68
2:D:59:PHE:HZ	2:D:108:ILE:HG21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD13	1:A:300:ALA:HB3	1.76	0.68
2:B:52:ALA:HB1	2:B:163:ALA:HB1	1.76	0.68
1:A:262:ILE:CD1	1:A:300:ALA:HB3	2.24	0.68
1:C:370:ILE:HD13	1:C:382:VAL:CG2	2.24	0.68
1:C:485:THR:HG23	1:C:486:ASN:N	2.09	0.67
1:C:426:ASP:CB	1:C:489:VAL:HG13	2.25	0.67
1:A:42:THR:HG21	1:A:46:GLY:C	2.15	0.67
1:C:269:TYR:O	1:C:273:ALA:HB2	1.93	0.67
1:C:428:ASN:HB2	1:C:429:ILE:HD12	1.77	0.67
1:C:77:ILE:H	1:C:77:ILE:HD12	1.59	0.67
1:C:35:PHE:CZ	1:C:39:ILE:HD12	2.31	0.66
2:D:283:ARG:HG2	2:D:381:GLU:CG	2.26	0.66
1:A:485:THR:HG23	1:A:486:ASN:N	2.10	0.65
1:A:203:ILE:HD12	1:A:232:ILE:CD1	2.25	0.65
2:B:361:ALA:HB2	2:B:377:GLU:HB3	1.78	0.65
1:C:215:PHE:CE1	1:C:285:MET:CA	2.77	0.65
1:A:448:ARG:HG3	1:A:449:GLY:N	2.06	0.65
2:D:361:ALA:HB2	2:D:377:GLU:HB3	1.79	0.65
1:A:266:ASP:OD1	1:A:322:GLU:HA	1.96	0.65
2:D:79:LEU:HD12	2:D:80:PRO:HD2	1.78	0.65
1:A:64:ALA:HB3	1:A:65:PRO:HD3	1.77	0.65
2:D:127:GLN:HB3	2:D:130:VAL:O	1.96	0.65
2:B:274:VAL:HG11	2:B:364:ILE:HD13	1.79	0.64
2:B:364:ILE:N	2:B:364:ILE:HD12	2.12	0.64
1:C:485:THR:HG23	1:C:486:ASN:H	1.63	0.64
2:D:4:VAL:HG12	2:D:26:LEU:HD12	1.80	0.64
1:C:130:LYS:HE2	1:C:183:ARG:HA	1.79	0.64
1:C:133:GLY:CA	1:C:179:ARG:HH12	2.11	0.64
1:C:429:ILE:HD12	1:C:429:ILE:N	2.13	0.64
1:C:159:PHE:O	1:C:201:GLU:HA	1.98	0.64
1:C:222:TYR:CE1	1:C:224:GLU:HB2	2.33	0.64
2:B:127:GLN:HG3	2:B:129:PRO:HD2	1.80	0.64
1:A:392:ASN:C	1:A:392:ASN:HD22	2.01	0.63
1:A:399:ILE:HD13	1:A:400:GLU:N	2.13	0.63
1:C:130:LYS:CE	1:C:183:ARG:HA	2.28	0.63
1:A:42:THR:HB	1:A:46:GLY:HA2	1.80	0.63
1:C:39:ILE:HD11	1:C:106:PHE:CD2	2.32	0.63
1:A:308:SER:CA	1:A:311:LEU:HD23	2.26	0.63
1:C:385:ASN:C	1:C:385:ASN:HD22	2.00	0.63
1:C:35:PHE:CE2	1:C:39:ILE:HD12	2.33	0.63
1:C:426:ASP:HB2	1:C:489:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LEU:HD12	2:B:80:PRO:CD	2.29	0.63
1:C:47:LEU:HD21	1:C:107:ARG:CZ	2.29	0.62
2:D:75:ARG:HG3	2:D:75:ARG:HH11	1.64	0.62
1:A:399:ILE:HD13	1:A:399:ILE:C	2.20	0.62
2:D:141:VAL:CG1	2:D:253:ILE:HD13	2.29	0.62
1:C:370:ILE:HD12	1:C:385:ASN:HB3	1.79	0.62
1:A:31:THR:HB	1:A:88:ASN:HD21	1.62	0.62
2:B:290:PRO:HD3	2:B:351:VAL:HG13	1.82	0.62
1:C:282:ARG:HG2	1:C:282:ARG:HH11	1.64	0.62
2:B:4:VAL:HG12	2:B:26:LEU:HD12	1.80	0.62
1:C:178:LEU:CD1	1:C:236:ILE:HD12	2.30	0.62
2:D:290:PRO:HD3	2:D:351:VAL:HG13	1.82	0.62
1:A:485:THR:HG23	1:A:486:ASN:H	1.65	0.61
2:B:127:GLN:HB3	2:B:130:VAL:O	2.00	0.61
2:B:314:GLY:H	2:B:319:ARG:HA	1.64	0.61
2:B:34:PRO:O	2:B:130:VAL:HG21	2.00	0.61
1:A:232:ILE:O	1:A:236:ILE:HG12	2.01	0.61
2:D:34:PRO:HG2	2:D:130:VAL:HB	1.83	0.61
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.65	0.61
1:C:130:LYS:NZ	1:C:183:ARG:HA	2.15	0.61
1:C:399:ILE:HD13	1:C:399:ILE:C	2.21	0.60
1:C:232:ILE:O	1:C:236:ILE:HG13	2.01	0.60
2:D:125:PRO:O	2:D:126:GLN:O	2.18	0.60
1:A:386:PHE:CE2	1:A:442:PRO:HG3	2.36	0.60
2:B:283:ARG:HG2	2:B:381:GLU:CG	2.31	0.60
1:C:426:ASP:CG	1:C:429:ILE:HD13	2.20	0.60
2:D:113:LEU:C	2:D:113:LEU:HD12	2.21	0.60
1:A:319:THR:C	1:A:321:GLY:H	2.05	0.60
1:C:49:LEU:HB3	1:C:80:LEU:HD22	1.83	0.60
1:A:142:GLU:HG2	1:A:192:LEU:CD2	2.31	0.60
2:B:34:PRO:HG2	2:B:130:VAL:HB	1.84	0.60
2:B:272:PRO:HB3	2:B:300:PHE:HB3	1.83	0.59
1:C:410:LYS:HD3	2:D:237:TRP:CZ3	2.37	0.59
1:C:261:LEU:C	1:C:261:LEU:HD23	2.23	0.59
1:C:375:ASP:O	1:C:376:GLY:O	2.20	0.59
2:B:115:LEU:C	2:B:115:LEU:HD23	2.22	0.59
1:C:77:ILE:HG22	1:C:78:VAL:HG23	1.84	0.59
1:A:385:ASN:C	1:A:385:ASN:HD22	2.06	0.59
1:C:156:ILE:HD11	1:C:182:TYR:HB3	1.84	0.59
2:D:115:LEU:HD23	2:D:115:LEU:C	2.23	0.59
1:A:375:ASP:O	1:A:376:GLY:O	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:SER:CA	1:C:311:LEU:HD23	2.30	0.59
2:B:190:HIS:ND1	2:B:191:LEU:HG	2.18	0.59
1:C:133:GLY:H	1:C:179:ARG:HH12	1.50	0.59
1:A:159:PHE:O	1:A:201:GLU:HA	2.03	0.58
1:C:382:VAL:H	1:C:385:ASN:HD21	1.50	0.58
1:A:68:GLU:O	1:A:72:THR:HG22	2.03	0.58
1:C:413:GLU:HB3	1:C:414:PRO:HD3	1.85	0.58
1:C:386:PHE:CE2	1:C:442:PRO:HG3	2.39	0.58
1:C:32:ASP:OD2	1:C:88:ASN:HB3	2.04	0.58
1:C:370:ILE:HD13	1:C:382:VAL:HG21	1.85	0.58
1:A:132:ALA:O	1:A:133:GLY:O	2.22	0.57
1:A:165:SER:OG	1:A:168:HIS:HB2	2.04	0.57
2:B:75:ARG:HG3	2:B:75:ARG:HH11	1.68	0.57
2:B:352:THR:CG2	2:B:354:GLU:HG2	2.34	0.57
2:D:141:VAL:HG13	2:D:253:ILE:HD13	1.85	0.57
1:A:39:ILE:HG13	1:A:39:ILE:O	2.04	0.57
1:A:340:GLU:OE2	1:A:351:ARG:NH1	2.37	0.57
1:A:42:THR:CG2	1:A:43:GLY:N	2.68	0.57
1:C:68:GLU:O	1:C:72:THR:HG22	2.04	0.57
1:C:192:LEU:HD22	1:C:192:LEU:H	1.69	0.57
1:A:426:ASP:CB	1:A:489:VAL:HG13	2.34	0.57
2:B:186:TRP:CE2	2:B:236:PHE:HB2	2.39	0.57
2:D:60:ARG:HA	2:D:60:ARG:NH1	2.18	0.57
1:A:222:TYR:CE1	1:A:224:GLU:HB2	2.40	0.57
2:B:125:PRO:O	2:B:126:GLN:O	2.22	0.57
2:D:283:ARG:HG2	2:D:381:GLU:HG2	1.87	0.57
2:D:84:LYS:O	2:D:84:LYS:HD3	2.04	0.57
1:C:136:SER:OG	1:C:186:HIS:HD2	1.88	0.56
1:C:178:LEU:HD13	1:C:236:ILE:HD12	1.85	0.56
2:D:186:TRP:CE2	2:D:236:PHE:HB2	2.40	0.56
2:D:190:HIS:ND1	2:D:191:LEU:HG	2.19	0.56
1:A:431:ILE:N	1:A:431:ILE:HD12	2.21	0.56
1:A:49:LEU:HB3	1:A:80:LEU:HD22	1.87	0.56
2:B:113:LEU:C	2:B:113:LEU:HD12	2.26	0.56
2:D:272:PRO:HB3	2:D:300:PHE:HB3	1.87	0.56
1:C:489:VAL:HG22	1:C:489:VAL:O	2.05	0.56
1:C:205:LEU:HD11	1:C:240:ILE:HG22	1.88	0.56
2:B:41:ASP:OD2	2:B:43:GLU:HB2	2.07	0.55
1:A:366:LYS:NZ	2:B:207:GLN:HE22	2.04	0.55
2:B:41:ASP:HB3	2:B:43:GLU:H	1.71	0.55
1:A:261:LEU:C	1:A:261:LEU:HD23	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HD11	1:C:106:PHE:CG	2.42	0.55
2:D:160:LEU:N	2:D:235:THR:HG22	2.13	0.55
1:A:42:THR:HG21	1:A:47:LEU:H	1.61	0.55
1:C:385:ASN:HD22	1:C:386:PHE:N	2.05	0.55
2:D:50:ASP:HB3	2:D:56:GLN:HG3	1.87	0.55
2:D:151:ARG:HH12	2:D:271:PRO:HG3	1.72	0.55
1:C:139:LEU:HB2	1:C:187:THR:HB	1.88	0.55
1:C:32:ASP:N	1:C:88:ASN:HD22	1.86	0.55
1:C:63:LEU:HD22	1:C:67:TYR:HB2	1.90	0.55
1:C:47:LEU:HD21	1:C:107:ARG:NH1	2.22	0.54
2:D:342:LEU:C	2:D:342:LEU:HD23	2.27	0.54
1:A:93:ASN:ND2	2:B:97:ARG:NH1	2.54	0.54
1:C:156:ILE:N	1:C:156:ILE:HD12	2.23	0.54
1:C:481:GLN:HA	1:C:488:PRO:HG3	1.89	0.54
2:B:168:THR:HG21	1:C:168:HIS:HB3	1.87	0.54
2:D:28:ARG:NH2	2:D:34:PRO:HB3	2.22	0.54
1:C:133:GLY:CA	1:C:134:PRO:C	2.76	0.54
1:C:343:SER:C	1:C:345:ASP:H	2.10	0.54
2:B:60:ARG:HA	2:B:60:ARG:NH1	2.19	0.54
2:B:85:TRP:CD1	2:B:85:TRP:C	2.81	0.54
2:B:50:ASP:HB3	2:B:56:GLN:HG3	1.90	0.54
2:B:235:THR:HG21	4:B:2027:HOH:O	2.07	0.54
1:A:32:ASP:OD2	1:A:88:ASN:HB3	2.07	0.53
1:A:139:LEU:HB2	1:A:187:THR:HB	1.89	0.53
2:B:352:THR:HG22	2:B:354:GLU:HG2	1.90	0.53
1:C:142:GLU:HG2	1:C:192:LEU:CD2	2.32	0.53
2:D:34:PRO:HG2	2:D:130:VAL:CB	2.38	0.53
1:C:100:TYR:CZ	2:D:97:ARG:HG3	2.43	0.53
1:A:136:SER:OG	1:A:186:HIS:HD2	1.90	0.53
2:B:198:LEU:HD23	2:B:199:ALA:N	2.23	0.53
1:C:428:ASN:C	1:C:429:ILE:HD12	2.28	0.53
2:D:352:THR:CG2	2:D:354:GLU:HG2	2.39	0.53
2:B:41:ASP:HB3	2:B:43:GLU:N	2.23	0.53
1:C:288:LYS:HG2	1:C:292:ASP:OD2	2.09	0.53
2:D:79:LEU:HD12	2:D:80:PRO:CD	2.39	0.53
2:B:167:PRO:HG3	1:C:164:PHE:CZ	2.43	0.53
2:D:218:PHE:CG	3:D:1233:NAG:H62	2.44	0.53
2:B:274:VAL:HG11	2:B:364:ILE:CD1	2.38	0.53
1:C:392:ASN:HD22	1:C:392:ASN:C	2.10	0.53
2:B:243:PRO:O	2:B:246:GLU:HB2	2.09	0.53
1:A:63:LEU:HD22	1:A:67:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:HB3	1:A:414:PRO:HD3	1.90	0.52
1:A:425:LYS:HE3	1:A:491:GLN:NE2	2.24	0.52
1:A:426:ASP:HB2	1:A:489:VAL:HG13	1.90	0.52
2:B:79:LEU:CD1	2:B:80:PRO:HD2	2.36	0.52
1:A:42:THR:HG23	1:A:47:LEU:O	2.09	0.52
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.73	0.52
1:A:485:THR:HG23	1:A:486:ASN:ND2	2.24	0.52
1:A:201:GLU:O	1:A:201:GLU:HG3	2.09	0.52
1:A:448:ARG:CG	1:A:449:GLY:H	2.08	0.52
2:B:283:ARG:HG2	2:B:381:GLU:HG2	1.92	0.52
1:C:473:LEU:O	1:C:477:ILE:HG12	2.09	0.52
1:A:343:SER:C	1:A:345:ASP:H	2.12	0.52
1:C:77:ILE:HD12	1:C:77:ILE:N	2.24	0.52
1:C:131:GLN:C	1:C:133:GLY:H	2.13	0.52
1:A:288:LYS:HG2	1:A:292:ASP:OD2	2.10	0.51
1:A:473:LEU:O	1:A:477:ILE:HG12	2.09	0.51
1:C:119:ARG:HG2	1:C:119:ARG:NH1	2.22	0.51
1:A:192:LEU:H	1:A:192:LEU:HD22	1.76	0.51
1:A:489:VAL:O	1:A:489:VAL:HG22	2.09	0.51
2:D:85:TRP:CD1	2:D:85:TRP:C	2.84	0.51
2:B:170:GLU:HA	4:B:2047:HOH:O	2.11	0.51
1:C:131:GLN:O	1:C:179:ARG:NH1	2.43	0.51
2:D:127:GLN:HG3	2:D:129:PRO:HD2	1.93	0.51
1:A:488:PRO:HB2	1:A:490:ILE:HD11	1.92	0.51
1:C:215:PHE:CD2	1:C:284:MET:HB2	2.46	0.51
1:C:130:LYS:HZ3	1:C:183:ARG:HA	1.75	0.51
1:C:192:LEU:HD22	1:C:192:LEU:N	2.26	0.51
1:A:321:GLY:O	1:A:322:GLU:HB3	2.11	0.51
1:A:392:ASN:C	1:A:392:ASN:ND2	2.63	0.51
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.75	0.51
1:C:453:ILE:N	1:C:453:ILE:HD12	2.25	0.51
1:C:49:LEU:CB	1:C:80:LEU:HD22	2.41	0.51
2:D:164:TYR:OH	2:D:167:PRO:HD3	2.11	0.51
1:A:393:GLU:O	1:A:458:ALA:O	2.29	0.50
1:C:201:GLU:O	1:C:201:GLU:HG3	2.10	0.50
1:C:165:SER:OG	1:C:168:HIS:HB2	2.11	0.50
2:D:96:PRO:HD3	2:D:257:TYR:CE1	2.45	0.50
1:C:278:TYR:CE2	1:C:282:ARG:NH2	2.73	0.50
1:C:485:THR:HG23	1:C:486:ASN:ND2	2.26	0.50
1:C:53:PHE:HA	1:C:100:TYR:CD1	2.46	0.50
2:B:190:HIS:CE1	2:B:191:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ASP:OD2	2:B:225:GLU:HG2	2.11	0.50
1:C:133:GLY:HA3	1:C:134:PRO:C	2.32	0.50
2:D:151:ARG:HH12	2:D:271:PRO:CG	2.24	0.50
1:A:131:GLN:C	1:A:133:GLY:H	2.13	0.50
2:D:90:THR:O	2:D:90:THR:CG2	2.58	0.50
1:A:49:LEU:CB	1:A:80:LEU:HD22	2.42	0.50
1:A:322:GLU:HG2	4:A:2032:HOH:O	2.12	0.50
1:C:115:TYR:CZ	1:C:124:ILE:HD13	2.47	0.50
1:C:436:ALA:HB3	1:C:450:PHE:HE2	1.76	0.50
1:C:222:TYR:CZ	1:C:224:GLU:HB2	2.46	0.49
2:D:243:PRO:O	2:D:246:GLU:HB2	2.13	0.49
1:C:31:THR:HB	1:C:88:ASN:ND2	2.25	0.49
2:B:55:LEU:CD1	2:B:115:LEU:HD11	2.42	0.49
2:B:132:ILE:HD13	2:B:133:THR:H	1.73	0.49
1:C:429:ILE:N	1:C:429:ILE:CD1	2.75	0.49
1:C:485:THR:CG2	1:C:486:ASN:N	2.75	0.49
2:B:34:PRO:HG2	2:B:130:VAL:CG2	2.43	0.49
1:C:370:ILE:CD1	1:C:385:ASN:HB3	2.42	0.49
1:C:233:LYS:O	1:C:237:GLN:HG3	2.13	0.49
1:C:399:ILE:HD13	1:C:400:GLU:C	2.33	0.49
1:A:178:LEU:HD21	1:A:233:LYS:HD2	1.95	0.49
2:B:49:HIS:CE1	2:B:51:PRO:HG3	2.47	0.49
1:C:133:GLY:CA	1:C:134:PRO:O	2.61	0.49
2:D:4:VAL:HG12	2:D:26:LEU:CD1	2.42	0.49
1:A:47:LEU:HD21	1:A:107:ARG:CZ	2.43	0.49
2:B:4:VAL:HG12	2:B:26:LEU:CD1	2.43	0.49
1:C:243:ILE:CG1	1:C:244:CYS:N	2.71	0.49
1:C:426:ASP:CA	1:C:489:VAL:HG13	2.43	0.49
2:D:42:PRO:HG2	2:D:125:PRO:HB3	1.95	0.49
1:A:39:ILE:HD12	1:A:48:MET:SD	2.53	0.49
2:B:90:THR:O	2:B:90:THR:CG2	2.53	0.49
2:B:288:GLU:O	2:B:351:VAL:HG22	2.13	0.49
1:C:100:TYR:O	2:D:94:ASN:HB2	2.13	0.49
2:D:182:PHE:O	2:D:201:THR:HA	2.12	0.49
1:A:119:ARG:HG2	1:A:119:ARG:NH1	2.23	0.48
2:B:316:PRO:HD3	2:B:354:GLU:O	2.13	0.48
1:C:485:THR:CG2	1:C:486:ASN:H	2.26	0.48
1:C:393:GLU:O	1:C:458:ALA:O	2.30	0.48
2:D:352:THR:HG22	2:D:354:GLU:HG2	1.94	0.48
1:C:319:THR:O	1:C:321:GLY:N	2.46	0.48
2:B:283:ARG:HG3	2:B:283:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLY:H	1:C:179:ARG:NH1	2.10	0.48
2:D:110:SER:HB2	2:D:111:PRO:HD2	1.96	0.48
1:C:192:LEU:H	1:C:192:LEU:CD2	2.26	0.48
1:C:385:ASN:C	1:C:385:ASN:ND2	2.66	0.48
1:A:382:VAL:H	1:A:385:ASN:ND2	2.06	0.48
2:D:250:LEU:HD23	2:D:261:GLN:OE1	2.14	0.48
1:A:481:GLN:HA	1:A:488:PRO:HG3	1.95	0.48
1:C:156:ILE:CD1	1:C:182:TYR:HB3	2.43	0.48
2:D:182:PHE:CE1	2:D:202:PRO:HG2	2.49	0.48
2:B:96:PRO:HD3	2:B:257:TYR:CE1	2.49	0.48
2:B:315:GLY:C	2:B:317:GLY:H	2.16	0.48
2:D:190:HIS:CE1	2:D:191:LEU:HG	2.49	0.48
2:D:223:ASP:OD2	2:D:225:GLU:HG2	2.14	0.48
1:A:485:THR:CG2	1:A:486:ASN:N	2.77	0.47
1:A:485:THR:CG2	1:A:486:ASN:H	2.27	0.47
2:B:182:PHE:CE1	2:B:202:PRO:HG2	2.49	0.47
2:D:151:ARG:O	2:D:154:GLN:HB2	2.13	0.47
2:B:47:SER:CB	2:B:132:ILE:HD12	2.42	0.47
2:B:342:LEU:C	2:B:342:LEU:HD23	2.35	0.47
2:D:171:ALA:O	2:D:172:ALA:HB2	2.14	0.47
1:C:243:ILE:HG13	1:C:244:CYS:H	1.73	0.47
1:C:443:SER:HB3	1:C:444:PRO:HD3	1.95	0.47
2:B:182:PHE:O	2:B:201:THR:HA	2.15	0.47
2:B:287:GLY:C	2:B:350:PRO:HB3	2.34	0.47
1:A:30:LEU:HG	1:A:81:ALA:HB1	1.96	0.47
1:A:399:ILE:HD13	1:A:400:GLU:C	2.34	0.47
2:B:160:LEU:N	2:B:235:THR:HG22	2.18	0.47
2:B:250:LEU:HD23	2:B:261:GLN:OE1	2.14	0.47
2:D:41:ASP:HB3	2:D:43:GLU:N	2.30	0.47
1:A:133:GLY:HA2	1:A:179:ARG:HH12	1.80	0.47
1:C:215:PHE:CD2	1:C:284:MET:CB	2.98	0.47
2:D:113:LEU:HD12	2:D:113:LEU:O	2.14	0.47
1:A:426:ASP:HA	1:A:489:VAL:HG13	1.97	0.46
2:B:364:ILE:N	2:B:364:ILE:CD1	2.77	0.46
1:C:455:PHE:O	1:C:457:PRO:HD3	2.15	0.46
1:C:132:ALA:O	1:C:133:GLY:O	2.32	0.46
1:C:275:GLY:O	1:C:278:TYR:HB3	2.16	0.46
1:A:321:GLY:O	1:A:323:ILE:HD12	2.15	0.46
1:A:436:ALA:HB3	1:A:450:PHE:HE2	1.81	0.46
1:A:490:ILE:N	1:A:490:ILE:HD12	2.31	0.46
1:A:385:ASN:HD22	1:A:386:PHE:N	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:HD12	2:B:115:LEU:HD11	1.97	0.46
1:C:30:LEU:HG	1:C:81:ALA:HB1	1.97	0.46
1:C:213:ASN:HD22	1:C:215:PHE:H	1.62	0.46
1:A:227:MET:HG3	1:A:232:ILE:HD11	1.97	0.46
1:C:215:PHE:O	1:C:288:LYS:HE2	2.16	0.46
1:A:386:PHE:CD2	1:A:442:PRO:HG3	2.50	0.46
2:B:167:PRO:C	2:B:169:SER:H	2.19	0.46
1:C:240:ILE:HD13	1:C:240:ILE:N	2.31	0.46
1:A:53:PHE:HA	1:A:100:TYR:CD1	2.51	0.46
2:B:281:LEU:HD12	2:B:380:LEU:HD23	1.98	0.46
2:D:198:LEU:HD23	2:D:199:ALA:N	2.31	0.46
1:C:363:ARG:CZ	1:C:365:LEU:HD11	2.46	0.46
2:D:41:ASP:HB3	2:D:43:GLU:H	1.80	0.46
2:D:287:GLY:C	2:D:350:PRO:HB3	2.35	0.46
1:A:222:TYR:CZ	1:A:224:GLU:HB2	2.51	0.46
2:B:42:PRO:HG2	2:B:125:PRO:HB3	1.97	0.46
1:A:218:LYS:HG3	1:A:219:THR:HG23	1.97	0.45
1:C:139:LEU:HD13	1:C:145:PHE:HA	1.98	0.45
1:C:340:GLU:OE2	1:C:351:ARG:NH1	2.49	0.45
2:B:59:PHE:CZ	2:B:108:ILE:HG21	2.38	0.45
1:C:132:ALA:O	1:C:133:GLY:C	2.54	0.45
2:D:281:LEU:HG	2:D:378:VAL:HG21	1.97	0.45
2:D:288:GLU:O	2:D:351:VAL:HG22	2.16	0.45
1:A:42:THR:O	1:A:43:GLY:O	2.34	0.45
1:A:156:ILE:HD12	1:A:236:ILE:HD12	1.98	0.45
1:A:213:ASN:HD22	1:A:215:PHE:H	1.62	0.45
1:C:386:PHE:CD2	1:C:442:PRO:HG3	2.51	0.45
2:D:249:TYR:C	2:D:250:LEU:HD12	2.36	0.45
1:A:31:THR:HB	1:A:88:ASN:ND2	2.31	0.45
2:B:84:LYS:HD3	2:B:84:LYS:O	2.17	0.45
1:C:477:ILE:CG2	1:C:490:ILE:HD13	2.40	0.45
1:A:426:ASP:CA	1:A:489:VAL:HG13	2.46	0.45
2:B:91:PRO:HG2	2:B:92:ALA:H	1.82	0.45
1:C:319:THR:C	1:C:321:GLY:H	2.19	0.45
2:D:91:PRO:HG2	2:D:92:ALA:H	1.80	0.45
2:B:110:SER:HB2	2:B:111:PRO:HD2	1.99	0.45
1:C:156:ILE:CD1	1:C:183:ARG:O	2.65	0.45
1:A:156:ILE:HD13	1:A:205:LEU:HG	1.99	0.45
2:B:100:ASP:O	2:B:120:ARG:NH2	2.50	0.45
1:C:133:GLY:HA2	1:C:134:PRO:O	2.16	0.45
2:D:141:VAL:HG11	2:D:253:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:LYS:HE2	2:D:327:ARG:NH1	2.32	0.45
2:B:139:LEU:HD13	2:B:255:LEU:HD12	1.98	0.45
1:C:343:SER:C	1:C:345:ASP:N	2.70	0.45
1:C:426:ASP:HA	1:C:489:VAL:HG13	1.99	0.45
2:D:128:GLU:HB2	2:D:129:PRO:CD	2.47	0.45
2:D:186:TRP:CZ3	2:D:251:ALA:HB2	2.52	0.45
1:A:192:LEU:HD22	1:A:192:LEU:N	2.32	0.45
1:A:319:THR:C	1:A:321:GLY:N	2.69	0.45
2:D:276:LEU:HD23	2:D:295:CYS:HA	1.98	0.45
1:A:119:ARG:HH11	1:A:119:ARG:CG	2.26	0.44
2:D:242:GLN:HB3	2:D:244:PHE:CD1	2.52	0.44
1:A:240:ILE:N	1:A:240:ILE:HD13	2.33	0.44
2:B:83:ALA:HB1	2:B:85:TRP:CE3	2.52	0.44
1:C:73:ARG:HD2	1:C:125:VAL:HG11	1.99	0.44
1:C:213:ASN:HD21	1:C:216:GLU:HG2	1.82	0.44
1:C:319:THR:O	1:C:319:THR:HG22	2.17	0.44
2:D:88:GLY:O	2:D:204:LEU:HD21	2.17	0.44
2:D:100:ASP:O	2:D:120:ARG:NH2	2.50	0.44
2:B:306:LEU:HD13	2:B:307:GLU:N	2.31	0.44
2:D:6:GLU:CD	2:D:37:ARG:HH22	2.21	0.44
1:A:93:ASN:HD22	1:A:93:ASN:HA	1.63	0.44
1:A:205:LEU:HD11	1:A:240:ILE:HG22	2.00	0.44
2:D:55:LEU:CD1	2:D:115:LEU:HD11	2.48	0.44
2:D:349:PRO:HB3	4:D:2088:HOH:O	2.17	0.44
1:A:399:ILE:C	1:A:399:ILE:CD1	2.86	0.44
1:C:382:VAL:H	1:C:385:ASN:ND2	2.15	0.44
2:D:199:ALA:HB3	2:D:209:PRO:HD2	1.99	0.44
2:D:120:ARG:HD2	2:D:138:VAL:HG21	1.99	0.44
2:D:281:LEU:HD12	2:D:380:LEU:HD23	2.00	0.44
1:C:417:LYS:O	1:C:421:GLU:HG3	2.18	0.44
1:A:228:THR:O	1:A:232:ILE:HG12	2.17	0.44
2:B:130:VAL:HG12	2:B:131:LEU:N	2.33	0.44
1:C:282:ARG:HG2	1:C:282:ARG:NH1	2.31	0.44
1:A:49:LEU:HD12	1:A:128:LEU:HD11	2.00	0.43
1:A:32:ASP:HA	1:A:91:THR:HG23	2.00	0.43
1:A:73:ARG:HD2	1:A:125:VAL:HG11	2.00	0.43
2:D:80:PRO:HD3	2:D:257:TYR:CE2	2.53	0.43
2:D:283:ARG:HG3	2:D:283:ARG:HH11	1.81	0.43
1:A:54:ALA:HB2	1:A:100:TYR:CE2	2.53	0.43
1:A:385:ASN:C	1:A:385:ASN:ND2	2.69	0.43
2:D:83:ALA:HB1	2:D:85:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:PRO:CG	2:D:348:PRO:HB2	2.48	0.43
2:D:115:LEU:HD23	2:D:116:SER:N	2.34	0.43
1:C:130:LYS:NZ	1:C:184:PHE:N	2.59	0.43
1:C:330:THR:CG2	1:C:334:GLU:HB2	2.48	0.43
1:C:392:ASN:C	1:C:392:ASN:ND2	2.71	0.43
1:A:187:THR:OG1	1:A:189:VAL:HG23	2.18	0.43
2:B:168:THR:O	2:B:168:THR:HG22	2.18	0.43
2:B:34:PRO:HG2	2:B:130:VAL:CB	2.49	0.43
1:C:32:ASP:N	1:C:88:ASN:ND2	2.53	0.43
1:C:303:SER:HB3	1:C:306:THR:OG1	2.19	0.43
2:B:120:ARG:HD2	2:B:138:VAL:HG21	1.99	0.43
1:C:295:HIS:HB3	1:C:357:PHE:CE1	2.54	0.43
2:B:322:LYS:HE2	2:B:327:ARG:NH1	2.34	0.43
1:C:265:TYR:CE1	1:C:267:VAL:HG22	2.54	0.43
1:C:428:ASN:HB2	1:C:429:ILE:CD1	2.44	0.43
1:C:218:LYS:HB2	1:C:218:LYS:HE3	1.86	0.42
2:D:52:ALA:CB	2:D:163:ALA:HB1	2.47	0.42
1:C:38:ARG:O	1:C:38:ARG:HG3	2.18	0.42
1:C:205:LEU:HD11	1:C:240:ILE:CG2	2.48	0.42
2:D:303:SER:HB2	2:D:332:LEU:HD21	2.01	0.42
2:D:306:LEU:HD13	2:D:307:GLU:N	2.34	0.42
1:C:399:ILE:HD12	1:C:401:PHE:CE1	2.53	0.42
1:C:450:PHE:HA	1:C:451:PRO:HA	1.81	0.42
2:D:55:LEU:HD12	2:D:115:LEU:HD11	2.01	0.42
2:B:199:ALA:HB3	2:B:209:PRO:HD2	2.02	0.42
2:B:281:LEU:HG	2:B:378:VAL:HG21	2.02	0.42
1:C:461:LYS:HA	1:C:461:LYS:HD3	1.83	0.42
1:A:175:ALA:O	1:A:179:ARG:N	2.52	0.42
1:A:203:ILE:CD1	1:A:232:ILE:HD12	2.41	0.42
2:B:47:SER:N	2:B:132:ILE:CD1	2.79	0.42
1:C:275:GLY:O	1:C:278:TYR:N	2.52	0.42
1:C:319:THR:C	1:C:321:GLY:N	2.72	0.42
2:B:124:GLU:HA	2:B:125:PRO:HD3	1.86	0.42
1:C:32:ASP:HA	1:C:91:THR:HG23	2.02	0.42
1:C:156:ILE:HD13	1:C:183:ARG:O	2.19	0.42
1:C:278:TYR:CE1	1:C:282:ARG:NE	2.80	0.42
2:D:113:LEU:C	2:D:113:LEU:CD1	2.88	0.42
1:A:343:SER:C	1:A:345:ASP:N	2.72	0.42
2:B:165:MET:SD	2:B:229:PRO:HB3	2.60	0.42
1:C:419:LEU:O	1:C:423:LEU:HD23	2.20	0.42
1:A:115:TYR:CZ	1:A:117:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:CYS:HB3	1:A:284:MET:HG2	2.02	0.41
1:C:47:LEU:O	1:C:79:PRO:HD2	2.20	0.41
1:C:115:TYR:CZ	1:C:117:GLY:HA3	2.55	0.41
1:A:31:THR:OG1	1:A:33:ASP:HB3	2.20	0.41
1:A:32:ASP:N	1:A:88:ASN:ND2	2.57	0.41
1:A:423:LEU:CB	1:A:431:ILE:HD11	2.50	0.41
2:B:151:ARG:O	2:B:154:GLN:HB2	2.20	0.41
1:C:379:LYS:HB3	1:C:432:ALA:HB2	2.02	0.41
2:D:59:PHE:CZ	2:D:108:ILE:HG21	2.45	0.41
2:D:79:LEU:CD1	2:D:80:PRO:HD2	2.46	0.41
2:B:290:PRO:CG	2:B:348:PRO:HB2	2.49	0.41
1:C:54:ALA:HB2	1:C:100:TYR:CE2	2.56	0.41
2:B:1:GLY:HA3	2:B:59:PHE:O	2.20	0.41
2:D:327:ARG:HA	2:D:345:HIS:O	2.20	0.41
2:B:186:TRP:CZ3	2:B:251:ALA:HB2	2.56	0.41
2:B:191:LEU:C	2:B:193:LYS:H	2.23	0.41
2:B:255:LEU:O	2:B:256:PRO:C	2.55	0.41
2:B:277:MET:HA	2:B:278:PRO:C	2.39	0.41
1:C:175:ALA:O	1:C:179:ARG:HB3	2.20	0.41
1:C:213:ASN:ND2	1:C:215:PHE:HB2	2.35	0.41
2:D:277:MET:HA	2:D:278:PRO:C	2.40	0.41
2:D:98:ALA:HB1	2:D:167:PRO:HB3	2.02	0.41
2:D:177:PRO:O	2:D:226:PRO:O	2.38	0.41
1:A:156:ILE:CD1	1:A:205:LEU:HG	2.50	0.41
2:B:43:GLU:HG2	2:B:125:PRO:HG3	2.03	0.41
1:C:426:ASP:HA	1:C:489:VAL:CG1	2.51	0.41
2:D:114:SER:HB3	2:D:143:THR:CG2	2.51	0.41
1:A:417:LYS:O	1:A:421:GLU:HG3	2.21	0.41
1:A:443:SER:HB3	1:A:444:PRO:HD3	2.03	0.41
1:C:277:ASN:O	1:C:281:ASN:ND2	2.54	0.41
1:A:167:ALA:HB1	1:A:227:MET:SD	2.60	0.41
1:A:213:ASN:ND2	1:A:215:PHE:HB2	2.36	0.41
1:A:330:THR:CG2	1:A:334:GLU:HB2	2.51	0.41
2:B:6:GLU:CD	2:B:37:ARG:HH22	2.23	0.41
2:B:115:LEU:HD23	2:B:116:SER:N	2.35	0.41
2:B:276:LEU:HD23	2:B:295:CYS:HA	2.02	0.41
2:D:62:TYR:HA	2:D:63:PRO:HD3	1.88	0.41
1:A:321:GLY:O	1:A:322:GLU:CB	2.68	0.41
2:B:62:TYR:HA	2:B:63:PRO:HD3	1.92	0.41
1:C:77:ILE:H	1:C:77:ILE:CD1	2.32	0.41
1:C:265:TYR:CZ	1:C:267:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:GLU:O	1:C:319:THR:N	2.53	0.41
2:D:26:LEU:HD21	2:D:28:ARG:HE	1.85	0.41
1:A:47:LEU:O	1:A:79:PRO:HD2	2.21	0.40
1:C:245:PRO:HD2	1:C:299:PHE:O	2.21	0.40
2:D:281:LEU:HG	2:D:378:VAL:CG2	2.51	0.40
1:C:39:ILE:HG12	1:C:39:ILE:O	2.20	0.40
1:C:273:ALA:O	1:C:274:LYS:C	2.59	0.40
2:D:43:GLU:HG2	2:D:125:PRO:HG3	2.03	0.40
2:D:75:ARG:HH11	2:D:75:ARG:CG	2.31	0.40
1:C:107:ARG:NH2	1:C:131:GLN:HE21	2.20	0.40
1:C:240:ILE:HD13	1:C:240:ILE:H	1.87	0.40
1:C:399:ILE:C	1:C:399:ILE:CD1	2.87	0.40
1:A:233:LYS:O	1:A:237:GLN:HG3	2.22	0.40
1:A:265:TYR:CZ	1:A:267:VAL:HG22	2.56	0.40
2:B:242:GLN:HB3	2:B:244:PHE:CD1	2.56	0.40
2:D:28:ARG:HH21	2:D:34:PRO:HB3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	467/481 (97%)	432 (92%)	30 (6%)	5 (1%)	14 30
1	C	458/481 (95%)	418 (91%)	31 (7%)	9 (2%)	7 14
2	B	353/401 (88%)	329 (93%)	21 (6%)	3 (1%)	19 39
2	D	351/401 (88%)	331 (94%)	17 (5%)	3 (1%)	17 35
All	All	1629/1764 (92%)	1510 (93%)	99 (6%)	20 (1%)	13 27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	GLY
2	B	126	GLN
1	C	376	GLY
2	D	126	GLN
1	A	43	GLY
1	A	133	GLY
1	A	393	GLU
1	C	133	GLY
1	C	318	SER
1	C	320	ALA
1	C	393	GLU
2	D	129	PRO
2	B	129	PRO
1	C	270	GLU
1	C	272	ASN
2	D	299	HIS
2	B	316	PRO
1	C	443	SER
1	A	443	SER
1	C	333	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/413 (97%)	384 (96%)	18 (4%)	27	52
1	C	397/413 (96%)	379 (96%)	18 (4%)	27	52
2	B	291/316 (92%)	274 (94%)	17 (6%)	20	40
2	D	290/316 (92%)	273 (94%)	17 (6%)	19	39
All	All	1380/1458 (95%)	1310 (95%)	70 (5%)	24	46

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	63	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	72	THR
1	A	168	HIS
1	A	179	ARG
1	A	199	ASN
1	A	240	ILE
1	A	266	ASP
1	A	291	LEU
1	A	345	ASP
1	A	375	ASP
1	A	385	ASN
1	A	387	ASP
1	A	392	ASN
1	A	399	ILE
1	A	406	CYS
1	A	460	LYS
1	A	489	VAL
2	B	6	GLU
2	B	20	LYS
2	B	42	PRO
2	B	60	ARG
2	B	85	TRP
2	B	115	LEU
2	B	124	GLU
2	B	132	ILE
2	B	134	MET
2	B	154	GLN
2	B	196	LEU
2	B	242	GLN
2	B	259	GLN
2	B	306	LEU
2	B	342	LEU
2	B	359	ARG
2	B	374	ARG
1	C	49	LEU
1	C	63	LEU
1	C	72	THR
1	C	179	ARG
1	C	199	ASN
1	C	240	ILE
1	C	291	LEU
1	C	306	THR
1	C	323	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	345	ASP
1	C	354	GLN
1	C	375	ASP
1	C	385	ASN
1	C	387	ASP
1	C	392	ASN
1	C	399	ILE
1	C	406	CYS
1	C	489	VAL
2	D	6	GLU
2	D	20	LYS
2	D	42	PRO
2	D	44	LEU
2	D	60	ARG
2	D	85	TRP
2	D	115	LEU
2	D	124	GLU
2	D	134	MET
2	D	154	GLN
2	D	196	LEU
2	D	242	GLN
2	D	259	GLN
2	D	306	LEU
2	D	342	LEU
2	D	359	ARG
2	D	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	88	ASN
1	A	93	ASN
1	A	177	ASN
1	A	186	HIS
1	A	194	ASN
1	A	213	ASN
1	A	237	GLN
1	A	281	ASN
1	A	339	GLN
1	A	354	GLN
1	A	385	ASN
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	394	ASN
1	A	411	ASN
1	A	486	ASN
1	A	491	GLN
2	B	49	HIS
2	B	127	GLN
2	B	154	GLN
2	B	207	GLN
2	B	254	HIS
2	B	259	GLN
2	B	355	GLN
1	C	88	ASN
1	C	93	ASN
1	C	131	GLN
1	C	177	ASN
1	C	186	HIS
1	C	194	ASN
1	C	213	ASN
1	C	237	GLN
1	C	246	HIS
1	C	281	ASN
1	C	339	GLN
1	C	354	GLN
1	C	385	ASN
1	C	392	ASN
1	C	394	ASN
1	C	411	ASN
1	C	486	ASN
2	D	154	GLN
2	D	207	GLN
2	D	254	HIS
2	D	259	GLN
2	D	299	HIS
2	D	355	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	1233	2	14,14,15	0.54	0	17,19,21	1.04	2 (11%)
3	NAG	B	1233	2	14,14,15	0.76	0	17,19,21	0.97	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1233	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1233	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1233	NAG	C2-N2-C7	-2.87	118.82	122.90
3	B	1233	NAG	C2-N2-C7	-2.11	119.90	122.90
3	D	1233	NAG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1233	NAG	O7-C7-N2-C2
3	D	1233	NAG	C8-C7-N2-C2
3	D	1233	NAG	O7-C7-N2-C2
3	B	1233	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1233	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	469/481 (97%)	-0.06	4 (0%) 84 82	29, 54, 75, 94	0
1	C	462/481 (96%)	0.51	36 (7%) 13 9	43, 78, 107, 119	0
2	B	361/401 (90%)	0.23	16 (4%) 34 27	29, 50, 100, 130	0
2	D	361/401 (90%)	0.14	11 (3%) 50 43	30, 52, 98, 125	0
All	All	1653/1764 (93%)	0.21	67 (4%) 37 30	29, 58, 100, 130	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	VAL	6.6
1	C	152	LYS	6.1
1	C	215	PHE	6.1
2	B	127	GLN	5.8
1	C	490	ILE	5.5
2	B	168	THR	5.4
1	C	116	ASP	4.8
2	B	169	SER	4.7
2	B	40	LEU	4.5
1	C	487	PRO	4.4
1	C	214	LYS	4.4
2	D	314	GLY	4.4
2	B	227	TRP	4.3
1	C	425	LYS	4.2
2	B	128	GLU	4.0
1	C	266	ASP	4.0
1	C	377	PRO	3.7
2	B	45	TYR	3.7
1	C	423	LEU	3.6
2	D	283	ARG	3.6
1	C	271	LYS	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	429	ILE	3.5
1	C	274	LYS	3.5
2	B	319	ARG	3.3
1	C	304	ARG	3.2
2	B	132	ILE	3.2
1	C	486	ASN	3.2
2	B	64	ARG	3.2
1	C	199	ASN	3.1
2	B	126	GLN	3.1
2	D	127	GLN	3.1
1	C	267	VAL	3.1
2	D	353	THR	3.0
1	C	458	ALA	3.0
1	C	129	LYS	2.9
2	D	128	GLU	2.9
2	B	177	PRO	2.9
2	D	357	GLY	2.8
1	C	394	ASN	2.8
2	D	130	VAL	2.6
1	C	427	PRO	2.6
2	D	282	ALA	2.6
2	D	284	ALA	2.5
1	C	125	VAL	2.5
1	C	322	GLU	2.5
1	C	193	VAL	2.5
1	A	320	ALA	2.4
1	C	78	VAL	2.4
1	C	47	LEU	2.4
2	D	281	LEU	2.4
1	A	226	LYS	2.4
2	D	315	GLY	2.3
1	C	345	ASP	2.3
1	C	323	ILE	2.3
2	B	131	LEU	2.3
1	C	420	GLY	2.2
1	C	341	GLU	2.2
1	C	396	ASP	2.2
2	B	283	ARG	2.2
1	C	77	ILE	2.2
1	C	485	THR	2.1
1	C	269	TYR	2.1
1	A	448	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	71	ALA	2.1
1	A	234	LYS	2.1
1	C	143	GLU	2.1
2	B	35	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	1233	14/15	0.93	0.15	53,56,61,62	0
3	NAG	D	1233	14/15	0.93	0.17	59,61,65,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.