Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2023 – 06:52 AM EST

PDB ID	:	1V9D
Title	:	Crystal structure of the core FH2 domain of mouse mDia1
Authors	:	Shimada, A.; Nyitrai, M.; Vetter, I.R.; Kuhlmann, D.; Bugyi, B.; Narumiya, S.; Geeves, M.A.; Wittinghofer, A.
Deposited on	:	2004-01-24
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

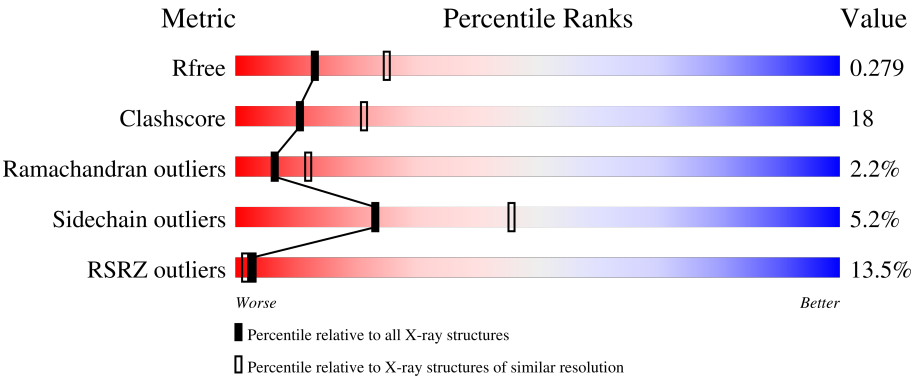
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 >=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 <=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	340	10% 55% 32% • 9%
1	B	340	5% 69% 23% • 6%
1	C	340	12% 48% 30% • 18%
1	D	340	21% 53% 32% • • 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10079 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.

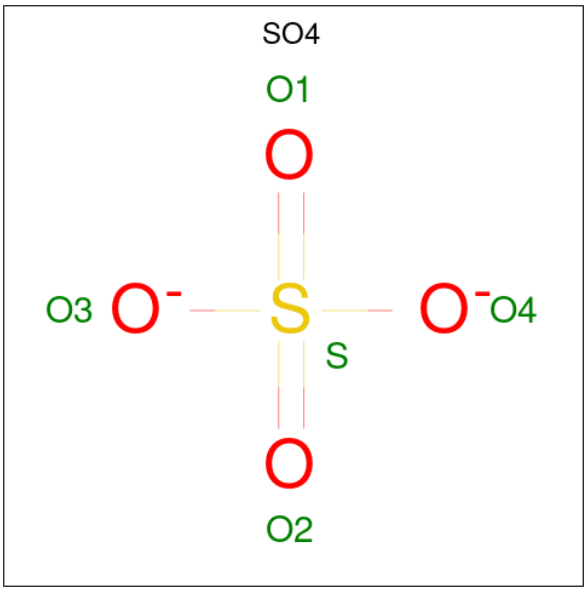
- Molecule 1 is a protein called Diaphanous protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2524	1595	428	484	17			
1	B	321	Total	C	N	O	S	0	0	0
			2611	1651	442	500	18			
1	C	278	Total	C	N	O	S	0	0	0
			2279	1444	384	435	16			
1	D	300	Total	C	N	O	S	0	0	0
			2458	1554	414	473	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	824	GLY	-	cloning artifact	UNP O08808
A	825	SER	-	cloning artifact	UNP O08808
B	824	GLY	-	cloning artifact	UNP O08808
B	825	SER	-	cloning artifact	UNP O08808
C	824	GLY	-	cloning artifact	UNP O08808
C	825	SER	-	cloning artifact	UNP O08808
D	824	GLY	-	cloning artifact	UNP O08808
D	825	SER	-	cloning artifact	UNP O08808

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

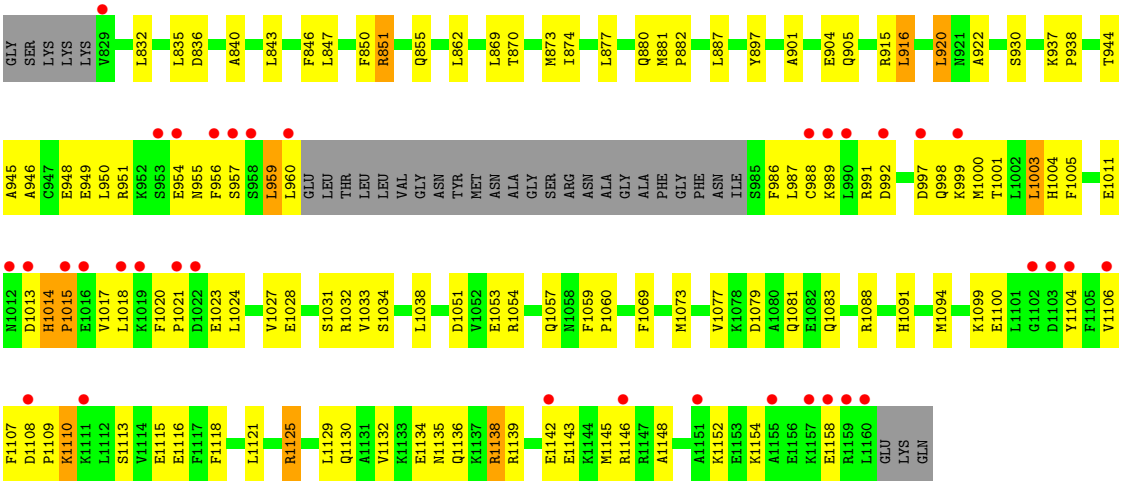
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	97	Total O 97 97	0	0
3	C	18	Total O 18 18	0	0
3	D	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

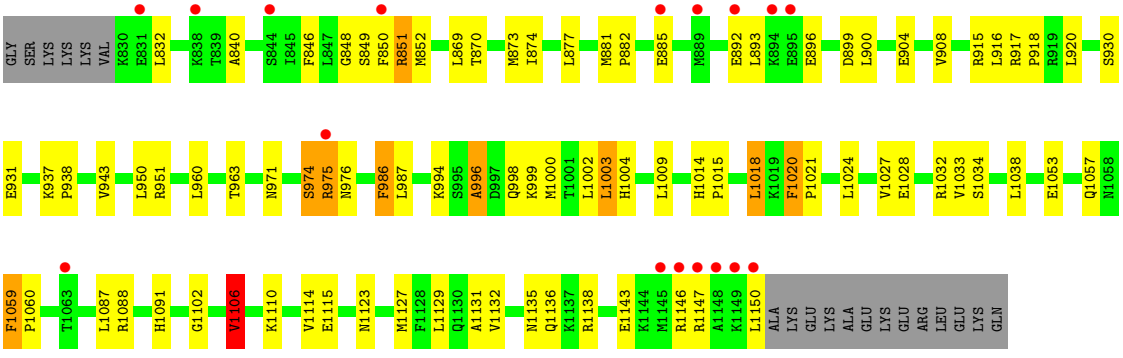
• Molecule 1: Diaphanous protein homolog 1

Chain A:



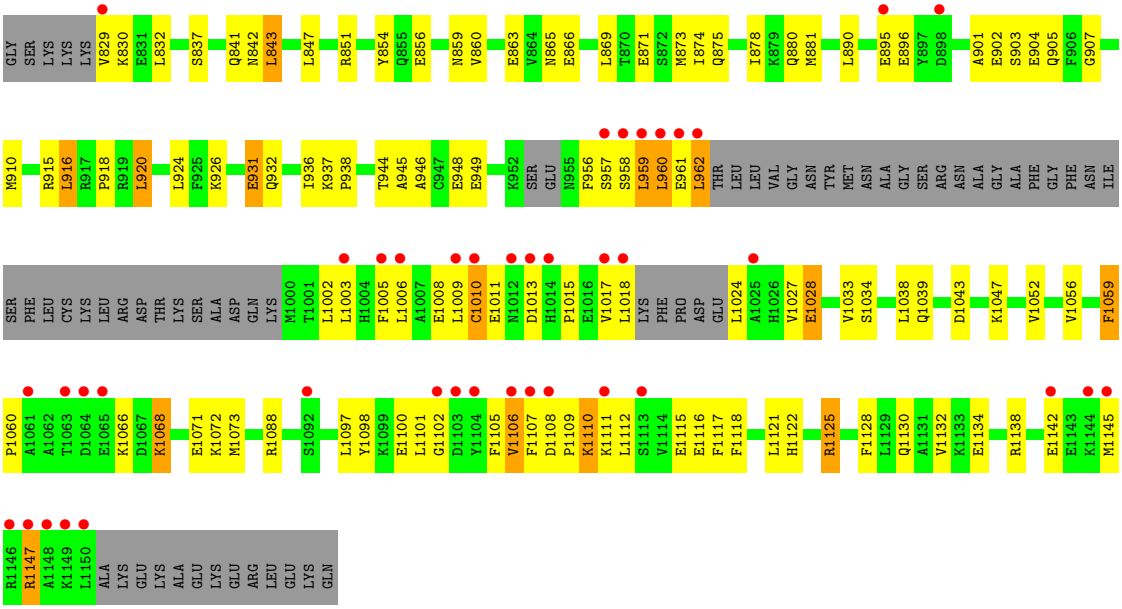
• Molecule 1: Diaphanous protein homolog 1

Chain B:



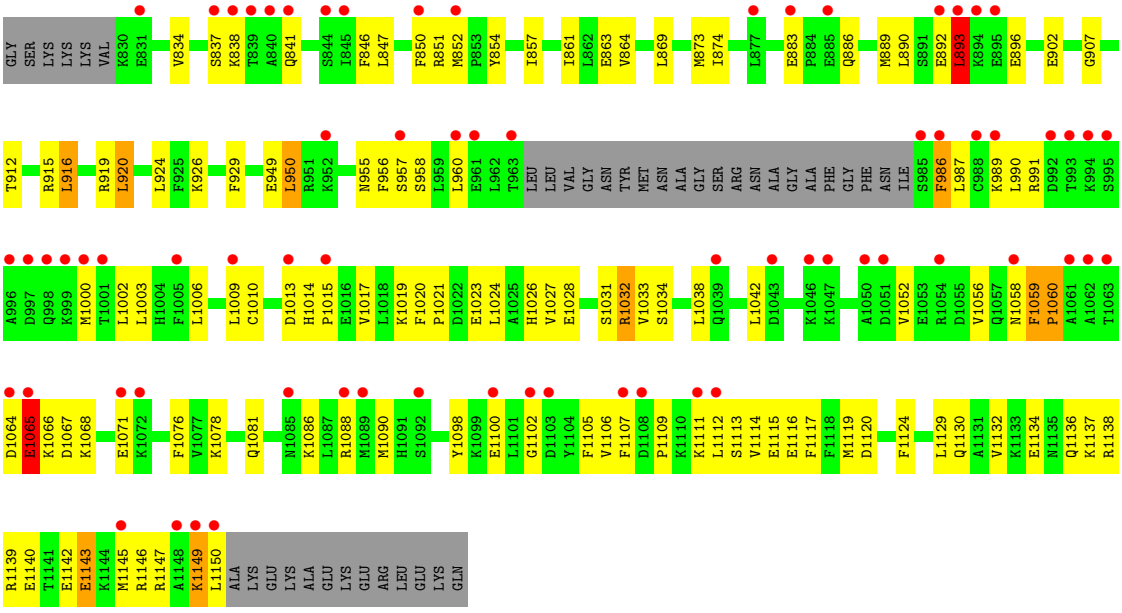
• Molecule 1: Diaphanous protein homolog 1

Chain C:



• Molecule 1: Diaphanous protein homolog 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.43Å 124.52Å 229.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 2.60 29.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.12-2.60) 96.1 (29.12-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.47 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.267 0.264 , 0.279	Depositor DCC
R_{free} test set	7136 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10079	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.38	0/2560	0.57	0/3427
1	B	0.40	0/2651	0.59	0/3555
1	C	0.32	0/2310	0.53	0/3094
1	D	0.30	0/2494	0.50	0/3342
All	All	0.35	0/10015	0.55	0/13418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2524	0	2555	107	0
1	B	2611	0	2627	63	0
1	C	2279	0	2303	103	0
1	D	2458	0	2479	95	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	69	0	0	11	0
3	B	97	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	18	0	0	5	0
3	D	8	0	0	0	0
All	All	10079	0	9964	365	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 18.

All (365) 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:C:962:LEU:HD23	1:C:962:LEU:H	1.30	0.93
1:A:1014:HIS:H	1:A:1015:PRO:HD3	1.33	0.92
1:A:1001:THR:HG22	1:A:1003:LEU:H	1.36	0.90
1:C:1108:ASP:HB3	1:C:1111:LYS:HB2	1.56	0.85
1:A:869:LEU:HD22	1:A:874:ILE:HD11	1.60	0.84
1:A:850:PHE:HB3	3:A:168:HOH:O	1.79	0.82
1:C:1138:ARG:O	1:C:1142:GLU:HG2	1.81	0.80
1:A:1001:THR:HB	1:A:1004:HIS:ND1	1.97	0.80
1:D:1107:PHE:O	1:D:1109:PRO:HD3	1.83	0.79
1:A:1014:HIS:N	1:A:1015:PRO:HD3	1.97	0.79
1:B:996:ALA:HA	3:B:179:HOH:O	1.83	0.78
1:C:1125:ARG:HB3	1:C:1125:ARG:NH1	1.99	0.77
1:A:869:LEU:HD23	1:A:873:MET:HE1	1.69	0.75
1:D:991:ARG:HB2	1:D:1003:LEU:HD12	1.67	0.75
1:D:1032:ARG:HG2	1:D:1032:ARG:HH11	1.51	0.74
1:B:1138:ARG:HB3	1:B:1138:ARG:NH1	2.03	0.73
1:A:1138:ARG:O	1:A:1142:GLU:HG2	1.88	0.73
1:A:956:PHE:HB2	1:A:1020:PHE:CE1	2.23	0.73
1:A:881:MET:CE	1:A:887:LEU:HD11	2.20	0.72
1:A:1125:ARG:NH1	1:A:1125:ARG:HB3	2.05	0.71
1:C:895:GLU:HG3	1:C:896:GLU:H	1.55	0.71
1:A:1018:LEU:O	1:A:1018:LEU:HD23	1.91	0.71
1:A:1028:GLU:HG2	1:A:1032:ARG:HH21	1.56	0.70
1:B:1123:ASN:O	1:B:1127:MET:HG2	1.91	0.70
1:C:1107:PHE:O	1:C:1109:PRO:HD3	1.91	0.70
1:C:1068:LYS:HA	1:C:1071:GLU:OE1	1.90	0.70
1:A:1125:ARG:HB3	1:A:1125:ARG:HH11	1.57	0.70
1:C:1013:ASP:C	1:C:1015:PRO:HD3	2.13	0.69
1:D:915:ARG:NH1	1:D:1060:PRO:HD3	2.07	0.69
1:C:916:LEU:HD22	1:C:920:LEU:HD22	1.73	0.69
1:D:1024:LEU:HB3	1:D:1027:VAL:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:LEU:O	1:C:1101:LEU:HD23	1.94	0.68
1:B:1138:ARG:HB3	1:B:1138:ARG:HH11	1.58	0.68
1:A:1115:GLU:HA	3:A:195:HOH:O	1.93	0.68
1:B:915:ARG:HB3	1:B:918:PRO:HG2	1.76	0.68
1:C:915:ARG:HB3	1:C:918:PRO:HG2	1.76	0.68
1:A:869:LEU:HD23	1:A:873:MET:CE	2.23	0.67
1:A:1113:SER:OG	1:A:1116:GLU:HG2	1.95	0.67
1:A:945:ALA:O	1:A:949:GLU:HG3	1.95	0.67
1:C:1018:LEU:HD22	1:C:1018:LEU:H	1.58	0.66
1:A:1031:SER:HA	3:A:195:HOH:O	1.93	0.66
1:C:961:GLU:CD	1:C:961:GLU:H	1.98	0.66
1:D:890:LEU:HD13	1:D:907:GLY:HA3	1.77	0.66
1:B:1000:MET:HG2	1:B:1004:HIS:HB2	1.77	0.66
1:D:950:LEU:HD13	1:D:1105:PHE:HE1	1.61	0.66
1:A:1020:PHE:HB3	1:A:1021:PRO:HD3	1.77	0.65
1:A:870:THR:HG22	1:B:930:SER:HB3	1.77	0.65
1:D:1014:HIS:N	1:D:1015:PRO:HD3	2.12	0.65
1:C:856:GLU:O	1:C:860:VAL:HG23	1.96	0.65
1:D:1136:GLN:O	1:D:1140:GLU:HB2	1.97	0.65
1:C:962:LEU:H	1:C:962:LEU:CD2	2.06	0.64
1:C:1102:GLY:O	1:C:1106:VAL:HA	1.98	0.64
1:C:1125:ARG:HB3	1:C:1125:ARG:HH11	1.60	0.64
1:D:863:GLU:OE1	1:D:1066:LYS:HD2	1.96	0.64
1:B:896:GLU:HB2	1:B:899:ASP:HB2	1.80	0.63
1:B:892:GLU:C	1:B:893:LEU:HD12	2.18	0.63
1:D:1068:LYS:HG3	1:D:1071:GLU:OE1	1.98	0.63
1:D:1024:LEU:HB3	1:D:1027:VAL:CG2	2.29	0.63
1:A:1108:ASP:OD1	1:A:1110:LYS:HE3	1.99	0.62
1:C:1145:MET:HE3	3:C:166:HOH:O	1.98	0.62
1:A:1132:VAL:O	1:A:1136:GLN:HG3	2.00	0.62
1:A:991:ARG:HB2	1:A:1003:LEU:HD12	1.80	0.62
1:C:1034:SER:HA	1:C:1115:GLU:CD	2.19	0.61
1:A:1130:GLN:HG3	1:A:1134:GLU:OE2	2.00	0.61
1:A:1023:GLU:O	1:A:1024:LEU:HD23	2.00	0.61
1:B:994:LYS:HD3	1:B:998:GLN:HB3	1.81	0.61
1:B:1135:ASN:HA	1:B:1138:ARG:HH12	1.66	0.61
1:C:869:LEU:HD23	1:C:873:MET:CE	2.30	0.61
1:D:1143:GLU:HA	1:D:1146:ARG:HH21	1.66	0.61
1:A:1077:VAL:O	1:A:1081:GLN:HG3	2.00	0.61
1:C:859:ASN:O	1:C:863:GLU:HG2	2.01	0.61
1:D:869:LEU:HD23	1:D:873:MET:CE	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:MET:HG2	1:A:1001:THR:H	1.66	0.60
1:D:956:PHE:O	1:D:960:LEU:HG	2.01	0.60
1:D:1031:SER:HB2	1:D:1119:MET:HA	1.82	0.60
1:B:1135:ASN:HA	1:B:1138:ARG:NH1	2.16	0.60
1:C:869:LEU:HD23	1:C:873:MET:HE1	1.84	0.60
1:B:869:LEU:HD23	1:B:873:MET:CE	2.32	0.60
1:D:1019:LYS:HB3	1:D:1019:LYS:NZ	2.17	0.60
1:A:881:MET:HE2	1:A:887:LEU:HD11	1.83	0.59
1:D:1014:HIS:O	1:D:1017:VAL:HG22	2.01	0.59
1:A:916:LEU:HD22	1:A:920:LEU:HD22	1.84	0.59
1:C:1147:ARG:C	1:C:1147:ARG:HD3	2.22	0.59
1:D:1130:GLN:O	1:D:1134:GLU:HG3	2.02	0.59
1:D:1033:VAL:O	1:D:1115:GLU:HB3	2.03	0.59
1:D:1147:ARG:HA	1:D:1150:LEU:HD13	1.84	0.59
1:A:944:THR:O	1:A:948:GLU:HG3	2.02	0.59
1:B:999:LYS:O	1:B:999:LYS:HG2	2.03	0.59
1:C:958:SER:O	1:C:959:LEU:HB2	2.01	0.59
1:A:991:ARG:HA	1:A:1001:THR:HG21	1.85	0.58
1:A:1033:VAL:HG12	1:A:1034:SER:N	2.19	0.58
1:D:1028:GLU:HG2	1:D:1032:ARG:HH21	1.69	0.58
1:B:848:GLY:C	1:B:850:PHE:H	2.05	0.58
1:C:1027:VAL:HG11	1:C:1121:LEU:HD12	1.85	0.58
1:A:1121:LEU:O	1:A:1121:LEU:HD13	2.03	0.58
1:D:1052:VAL:O	1:D:1056:VAL:HG23	2.03	0.58
1:C:1002:LEU:HD23	1:C:1002:LEU:O	2.03	0.57
1:C:1010:CYS:O	1:C:1015:PRO:HA	2.04	0.57
1:C:1039:GLN:HE22	1:C:1088:ARG:HH22	1.52	0.57
1:D:1002:LEU:O	1:D:1002:LEU:HD23	2.04	0.57
1:C:945:ALA:O	1:C:949:GLU:HG3	2.04	0.57
1:C:1147:ARG:HD3	1:C:1147:ARG:O	2.04	0.57
1:A:1023:GLU:HA	1:A:1023:GLU:OE1	2.03	0.57
1:B:846:PHE:O	1:B:850:PHE:HB2	2.05	0.57
1:C:1024:LEU:HG	3:C:127:HOH:O	2.04	0.57
1:C:1043:ASP:O	1:C:1047:LYS:HG2	2.04	0.57
1:D:846:PHE:O	1:D:850:PHE:HB2	2.04	0.57
1:A:881:MET:HE3	1:A:882:PRO:HD2	1.86	0.57
1:D:874:ILE:HG21	1:D:924:LEU:HB2	1.86	0.56
1:D:869:LEU:HD23	1:D:873:MET:HE1	1.86	0.56
1:A:1053:GLU:O	1:A:1057:GLN:HG3	2.06	0.56
1:A:1069:PHE:CE1	1:A:1073:MET:HG3	2.40	0.56
1:B:869:LEU:HD22	1:B:874:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:HIS:H	1:A:1015:PRO:CD	2.07	0.56
1:A:1146:ARG:HD2	3:A:89:HOH:O	2.05	0.56
1:D:1149:LYS:HD2	1:D:1149:LYS:C	2.26	0.56
1:A:955:ASN:O	1:A:959:LEU:HD13	2.05	0.56
1:B:986:PHE:HD2	1:B:986:PHE:O	1.88	0.56
1:C:937:LYS:HB3	1:C:938:PRO:HD3	1.88	0.56
1:C:895:GLU:HG3	1:C:896:GLU:N	2.21	0.55
1:D:1032:ARG:HG2	1:D:1032:ARG:NH1	2.22	0.55
1:A:1011:GLU:CD	1:A:1139:ARG:HH22	2.09	0.55
1:C:1121:LEU:HD13	1:C:1121:LEU:O	2.05	0.55
1:D:915:ARG:NH1	1:D:1059:PHE:HA	2.20	0.55
1:C:960:LEU:H	1:C:962:LEU:CD2	2.19	0.55
1:D:838:LYS:O	1:D:841:GLN:HB3	2.06	0.55
1:D:915:ARG:HH12	1:D:1059:PHE:HA	1.72	0.55
1:C:1024:LEU:N	3:C:127:HOH:O	2.39	0.55
1:C:1130:GLN:O	1:C:1134:GLU:HG3	2.07	0.54
1:D:950:LEU:HD13	1:D:1105:PHE:CE1	2.40	0.54
1:D:957:SER:HA	1:D:960:LEU:HD12	1.89	0.54
1:D:1088:ARG:HG3	1:D:1088:ARG:HH11	1.73	0.54
1:A:1118:PHE:HB2	3:A:195:HOH:O	2.07	0.54
1:B:1106:VAL:HG22	1:B:1106:VAL:O	2.07	0.53
1:A:1051:ASP:HA	1:A:1054:ARG:NH1	2.24	0.53
1:D:958:SER:HB2	1:D:1017:VAL:HG12	1.89	0.53
1:A:832:LEU:HD21	1:A:840:ALA:CB	2.39	0.53
1:C:1098:TYR:O	1:C:1101:LEU:HB2	2.09	0.53
1:A:1088:ARG:HH11	1:A:1088:ARG:HG3	1.74	0.53
1:A:881:MET:HE1	1:A:887:LEU:HD11	1.90	0.52
1:A:1021:PRO:HB3	1:A:1129:LEU:HD11	1.90	0.52
1:C:932:GLN:O	1:C:936:ILE:HG13	2.09	0.52
1:D:950:LEU:HD22	1:D:1105:PHE:CE1	2.43	0.52
1:B:1021:PRO:HG2	1:B:1129:LEU:HD21	1.91	0.52
1:D:1021:PRO:HG2	1:D:1129:LEU:HD21	1.90	0.52
1:C:1108:ASP:CB	1:C:1111:LYS:HB2	2.34	0.52
1:D:912:THR:O	1:D:912:THR:HG22	2.10	0.52
1:A:1107:PHE:O	1:A:1109:PRO:HD3	2.10	0.52
1:A:1021:PRO:HG2	1:A:1129:LEU:HD21	1.90	0.52
1:C:1028:GLU:HG2	1:C:1122:HIS:CE1	2.45	0.52
1:C:1009:LEU:C	1:C:1011:GLU:H	2.13	0.52
1:C:1018:LEU:HD22	1:C:1018:LEU:N	2.24	0.52
1:D:892:GLU:O	1:D:893:LEU:HB2	2.09	0.52
1:B:869:LEU:HD23	1:B:873:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1130:GLN:HG2	1:C:1134:GLU:OE2	2.11	0.51
1:D:915:ARG:CZ	1:D:1060:PRO:HD3	2.41	0.51
1:B:1033:VAL:HG12	1:B:1034:SER:N	2.25	0.51
1:C:960:LEU:C	1:C:960:LEU:HD23	2.31	0.51
1:D:1149:LYS:HE2	1:D:1150:LEU:CD1	2.40	0.51
1:B:885:GLU:H	1:B:885:GLU:CD	2.14	0.51
1:A:954:GLU:OE2	1:A:954:GLU:N	2.42	0.51
1:A:1024:LEU:HB3	1:A:1027:VAL:CG2	2.41	0.51
1:B:1143:GLU:HA	1:B:1146:ARG:HD3	1.92	0.51
1:C:842:ASN:HB3	1:C:880:GLN:HE22	1.76	0.51
1:D:1132:VAL:O	1:D:1136:GLN:HG3	2.11	0.51
1:A:1083:GLN:HA	1:A:1083:GLN:NE2	2.25	0.51
1:B:1033:VAL:CG1	1:B:1034:SER:N	2.73	0.51
1:D:1010:CYS:HA	1:D:1014:HIS:HB2	1.93	0.50
1:C:944:THR:O	1:C:948:GLU:HG3	2.11	0.50
1:A:987:LEU:HD13	1:A:987:LEU:O	2.12	0.50
1:D:1113:SER:OG	1:D:1116:GLU:HG3	2.11	0.50
1:D:850:PHE:CE1	1:D:852:MET:HB3	2.47	0.50
1:A:1033:VAL:CG1	1:A:1034:SER:N	2.74	0.50
1:C:1027:VAL:CG1	1:C:1121:LEU:HD12	2.42	0.50
1:B:1147:ARG:O	1:B:1150:LEU:HG	2.11	0.49
1:C:960:LEU:HD23	1:C:961:GLU:N	2.27	0.49
1:D:1139:ARG:HA	1:D:1142:GLU:HG2	1.93	0.49
1:A:1014:HIS:N	1:A:1015:PRO:CD	2.67	0.49
1:A:997:ASP:O	1:A:999:LYS:N	2.45	0.49
1:B:1102:GLY:O	1:B:1106:VAL:HA	2.13	0.49
1:C:869:LEU:HD22	1:C:874:ILE:HD11	1.92	0.49
1:B:937:LYS:HB3	1:B:938:PRO:HD3	1.94	0.49
1:C:960:LEU:H	1:C:962:LEU:HD23	1.77	0.49
1:C:1033:VAL:HG12	1:C:1034:SER:N	2.28	0.49
1:D:949:GLU:OE2	1:D:1026:HIS:ND1	2.43	0.49
1:D:986:PHE:HE2	1:D:989:LYS:HD3	1.78	0.49
1:A:1020:PHE:CB	1:A:1021:PRO:HD3	2.42	0.49
1:B:893:LEU:HD12	1:B:893:LEU:N	2.27	0.49
1:C:881:MET:HG2	1:C:916:LEU:HD13	1.95	0.49
1:D:987:LEU:HG	1:D:1124:PHE:CE1	2.47	0.49
1:C:946:ALA:HB1	1:C:1118:PHE:CE2	2.48	0.48
1:A:1024:LEU:HB3	1:A:1027:VAL:HG21	1.95	0.48
1:A:877:LEU:O	1:A:881:MET:HG2	2.13	0.48
1:A:1110:LYS:HD3	1:A:1110:LYS:N	2.29	0.48
1:A:1088:ARG:HG3	1:A:1088:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1014:HIS:N	1:D:1015:PRO:CD	2.76	0.48
1:A:847:LEU:HA	3:A:168:HOH:O	2.13	0.48
1:A:851:ARG:N	3:A:168:HOH:O	2.45	0.48
1:A:1154:LYS:HG2	1:A:1158:GLU:HG2	1.95	0.48
1:C:829:VAL:O	1:C:830:LYS:HB2	2.14	0.48
1:C:859:ASN:HB3	1:C:1066:LYS:HE3	1.96	0.48
1:C:874:ILE:O	1:C:878:ILE:HG13	2.14	0.48
1:A:851:ARG:HD3	3:A:45:HOH:O	2.13	0.48
1:D:847:LEU:O	1:D:850:PHE:HB3	2.13	0.48
1:D:916:LEU:HD22	1:D:920:LEU:HD22	1.95	0.48
1:D:1038:LEU:O	1:D:1042:LEU:HD13	2.14	0.48
1:A:937:LYS:HB3	1:A:938:PRO:HD3	1.95	0.48
1:D:1146:ARG:O	1:D:1149:LYS:HG3	2.13	0.48
1:A:862:LEU:HA	3:A:12:HOH:O	2.14	0.48
1:C:910:MET:HA	1:C:910:MET:CE	2.44	0.48
1:C:1039:GLN:NE2	1:C:1088:ARG:HH22	2.12	0.48
1:D:883:GLU:HB2	1:D:886:GLN:HE21	1.79	0.47
1:D:893:LEU:HD12	1:D:896:GLU:OE2	2.14	0.47
1:B:1053:GLU:HG2	1:B:1057:GLN:NE2	2.30	0.47
1:D:1065:GLU:O	1:D:1068:LYS:HE2	2.14	0.47
1:B:963:THR:HG21	1:B:987:LEU:HD21	1.96	0.47
1:A:1099:LYS:C	1:A:1099:LYS:HD3	2.35	0.47
1:D:1098:TYR:CD2	1:D:1114:VAL:HG22	2.50	0.47
1:A:835:LEU:HG	1:A:904:GLU:HG2	1.97	0.47
1:B:1091:HIS:HE1	3:B:11:HOH:O	1.97	0.47
1:C:1056:VAL:O	1:C:1059:PHE:HB2	2.14	0.47
1:D:1056:VAL:C	1:D:1058:ASN:H	2.18	0.47
1:A:1027:VAL:HG11	1:A:1121:LEU:HD12	1.96	0.47
1:C:1138:ARG:NH1	3:C:182:HOH:O	2.47	0.47
1:C:1147:ARG:C	1:C:1147:ARG:CD	2.83	0.47
1:D:834:VAL:HG13	1:D:889:MET:HE2	1.97	0.47
1:A:846:PHE:CG	1:A:880:GLN:HG3	2.50	0.47
1:C:837:SER:O	1:C:841:GLN:HG3	2.15	0.47
1:A:897:TYR:CZ	1:A:905:GLN:HB3	2.51	0.46
1:B:1003:LEU:HD13	1:B:1131:ALA:HB2	1.96	0.46
1:B:1024:LEU:HB3	1:B:1027:VAL:CG2	2.45	0.46
1:C:926:LYS:HB2	1:C:1073:MET:HE1	1.97	0.46
1:B:1015:PRO:O	1:B:1018:LEU:HB2	2.16	0.46
1:D:850:PHE:HE1	1:D:852:MET:SD	2.39	0.46
1:A:997:ASP:C	1:A:999:LYS:N	2.68	0.46
1:B:1138:ARG:HH11	1:B:1138:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1033:VAL:HG12	1:D:1034:SER:N	2.30	0.46
1:D:1067:ASP:C	1:D:1068:LYS:HD2	2.36	0.46
1:A:1059:PHE:HA	1:A:1060:PRO:HD3	1.83	0.46
1:A:1148:ALA:O	1:A:1152:LYS:HG3	2.16	0.46
1:A:922:ALA:HB1	1:A:1073:MET:CE	2.46	0.46
1:A:997:ASP:C	1:A:999:LYS:H	2.19	0.46
1:A:881:MET:HE3	1:A:882:PRO:CD	2.46	0.46
1:A:1004:HIS:HB3	1:A:1135:ASN:OD1	2.15	0.46
1:B:869:LEU:HD23	1:B:873:MET:HE2	1.97	0.46
1:C:830:LYS:HD3	1:C:901:ALA:HA	1.98	0.46
1:C:1011:GLU:C	1:C:1015:PRO:HG3	2.37	0.46
1:C:1142:GLU:HA	1:C:1142:GLU:OE2	2.16	0.46
1:D:1065:GLU:CD	1:D:1065:GLU:H	2.20	0.45
1:D:850:PHE:CD1	1:D:852:MET:HB3	2.51	0.45
1:A:960:LEU:HG	3:A:144:HOH:O	2.16	0.45
1:A:1091:HIS:O	1:A:1094:MET:HB3	2.16	0.45
1:B:971:ASN:HB3	1:B:974:SER:OG	2.15	0.45
1:C:901:ALA:O	1:C:905:GLN:HG3	2.15	0.45
1:C:1068:LYS:HB2	1:C:1072:LYS:HE2	1.99	0.45
1:D:854:TYR:OH	1:D:902:GLU:HB2	2.16	0.45
1:C:871:GLU:O	1:C:875:GLN:HG3	2.16	0.45
1:C:1112:LEU:HD12	1:C:1116:GLU:OE1	2.17	0.45
1:A:1033:VAL:O	1:A:1115:GLU:CG	2.65	0.45
1:D:1088:ARG:HG3	1:D:1088:ARG:NH1	2.31	0.45
1:D:1112:LEU:HD21	1:D:1117:PHE:HA	1.99	0.45
1:D:926:LYS:HA	1:D:1076:PHE:CE2	2.52	0.45
1:B:877:LEU:O	1:B:881:MET:HB2	2.17	0.45
1:D:1006:LEU:HD23	1:D:1010:CYS:HG	1.81	0.45
1:A:1033:VAL:O	1:A:1115:GLU:HG3	2.17	0.45
1:C:962:LEU:HD23	1:C:962:LEU:N	2.13	0.45
1:B:1014:HIS:N	1:B:1015:PRO:HD3	2.32	0.44
1:C:1008:GLU:O	1:C:1011:GLU:HB3	2.16	0.44
1:A:1013:ASP:O	1:A:1014:HIS:HB2	2.17	0.44
1:B:848:GLY:C	1:B:850:PHE:N	2.68	0.44
1:B:960:LEU:O	1:B:963:THR:HB	2.18	0.44
1:C:1039:GLN:HG3	1:C:1043:ASP:OD2	2.17	0.44
1:B:893:LEU:HD23	1:B:900:LEU:HD21	2.00	0.44
1:B:917:ARG:HG3	1:B:917:ARG:HH11	1.83	0.44
1:C:931:GLU:OE1	1:C:931:GLU:HA	2.17	0.44
1:D:1010:CYS:HB3	1:D:1017:VAL:CG2	2.48	0.44
1:D:1149:LYS:HE2	1:D:1150:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:SER:OG	1:B:870:THR:HG22	2.18	0.44
1:B:832:LEU:HD11	1:B:840:ALA:CB	2.48	0.44
1:C:1112:LEU:HD21	1:C:1117:PHE:HA	2.00	0.44
1:D:950:LEU:HD22	1:D:1105:PHE:CZ	2.53	0.44
1:B:1020:PHE:N	1:B:1021:PRO:CD	2.81	0.43
1:D:1138:ARG:C	1:D:1140:GLU:H	2.21	0.43
1:B:1088:ARG:HD3	3:B:112:HOH:O	2.18	0.43
1:D:1064:ASP:C	1:D:1066:LYS:H	2.21	0.43
1:C:1052:VAL:O	1:C:1056:VAL:HG23	2.18	0.43
1:A:1116:GLU:OE2	1:A:1116:GLU:HA	2.18	0.43
1:B:904:GLU:O	1:B:908:VAL:HG23	2.19	0.43
1:C:869:LEU:HD23	1:C:873:MET:HE2	2.00	0.43
1:D:1020:PHE:N	1:D:1021:PRO:CD	2.81	0.43
1:D:1078:LYS:O	1:D:1081:GLN:HB2	2.19	0.43
1:A:1017:VAL:HG12	1:A:1017:VAL:O	2.18	0.43
1:C:880:GLN:NE2	3:C:174:HOH:O	2.50	0.43
1:A:843:LEU:HD23	1:A:843:LEU:HA	1.83	0.43
1:A:1142:GLU:CB	1:A:1146:ARG:HH12	2.31	0.43
1:A:1154:LYS:O	1:A:1158:GLU:HG2	2.18	0.43
1:C:916:LEU:HD22	1:C:920:LEU:CD2	2.46	0.43
1:A:1021:PRO:HG2	1:A:1129:LEU:CD2	2.49	0.43
1:C:1106:VAL:O	1:C:1106:VAL:HG13	2.18	0.43
1:B:1020:PHE:CD1	1:B:1020:PHE:C	2.92	0.42
1:B:1132:VAL:O	1:B:1136:GLN:HG3	2.19	0.42
1:C:1018:LEU:H	1:C:1018:LEU:CD2	2.28	0.42
1:C:1108:ASP:HB3	1:C:1111:LYS:CB	2.38	0.42
1:D:1149:LYS:HG3	1:D:1150:LEU:HD12	2.01	0.42
1:A:901:ALA:O	1:A:905:GLN:HG3	2.19	0.42
1:C:895:GLU:CG	1:C:896:GLU:H	2.27	0.42
1:C:1110:LYS:HD3	1:C:1110:LYS:N	2.33	0.42
1:B:848:GLY:O	1:B:850:PHE:N	2.52	0.42
1:D:916:LEU:O	1:D:919:ARG:HB3	2.19	0.42
1:A:959:LEU:O	1:A:960:LEU:HG	2.19	0.42
1:A:986:PHE:C	1:A:988:CYS:N	2.73	0.42
1:A:991:ARG:HA	1:A:1001:THR:CG2	2.48	0.42
1:B:1033:VAL:O	1:B:1115:GLU:HB3	2.19	0.42
1:C:890:LEU:HD13	1:C:907:GLY:HA3	2.02	0.42
1:C:1003:LEU:HD22	1:C:1003:LEU:H	1.83	0.42
1:B:975:ARG:HG2	1:B:976:ASN:ND2	2.34	0.42
1:C:1128:PHE:O	1:C:1132:VAL:HG23	2.20	0.42
1:C:1002:LEU:CD2	1:C:1006:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ASP:CG	1:A:1110:LYS:HE3	2.40	0.42
1:C:902:GLU:HG3	1:C:903:SER:N	2.35	0.42
1:D:864:VAL:HG12	1:D:864:VAL:O	2.19	0.42
1:D:1068:LYS:HD2	1:D:1068:LYS:N	2.34	0.42
1:A:1145:MET:O	1:A:1148:ALA:HB3	2.19	0.42
1:C:874:ILE:HG21	1:C:924:LEU:HB2	2.02	0.42
1:C:1013:ASP:O	1:C:1015:PRO:HD3	2.19	0.42
1:A:946:ALA:HB1	1:A:1118:PHE:CE2	2.55	0.42
1:C:860:VAL:HG13	1:C:865:ASN:HB3	2.02	0.42
1:C:1109:PRO:C	1:C:1110:LYS:HD3	2.40	0.41
1:D:916:LEU:CD2	1:D:920:LEU:HD22	2.49	0.41
1:A:915:ARG:HG3	1:A:915:ARG:HH11	1.85	0.41
1:A:836:ASP:OD2	1:D:1137:LYS:HE3	2.20	0.41
1:C:926:LYS:HD2	1:C:1073:MET:HE2	2.01	0.41
1:C:1105:PHE:CD1	1:C:1105:PHE:N	2.88	0.41
1:D:857:ILE:O	1:D:861:ILE:HG13	2.21	0.41
1:D:987:LEU:HD11	1:D:990:LEU:HD11	2.02	0.41
1:B:915:ARG:NH1	1:B:1060:PRO:HD3	2.35	0.41
1:C:843:LEU:O	1:C:847:LEU:HG	2.20	0.41
1:A:951:ARG:HD2	1:A:1104:TYR:CE2	2.56	0.41
1:B:1024:LEU:HB3	1:B:1027:VAL:HG21	2.01	0.41
1:D:1086:LYS:O	1:D:1090:MET:HG3	2.20	0.41
1:B:881:MET:HA	1:B:882:PRO:HD3	1.95	0.41
1:B:917:ARG:HG3	1:B:917:ARG:NH1	2.35	0.41
1:B:1028:GLU:HG2	1:B:1032:ARG:HH21	1.85	0.41
1:B:1002:LEU:HA	1:B:1002:LEU:HD23	1.85	0.41
1:D:955:ASN:HD22	1:D:1023:GLU:CD	2.24	0.41
1:D:1056:VAL:C	1:D:1058:ASN:N	2.73	0.41
1:D:1059:PHE:HA	1:D:1060:PRO:HD3	1.85	0.41
1:A:1000:MET:HG2	1:A:1001:THR:N	2.31	0.41
1:A:1108:ASP:OD1	1:A:1110:LYS:HB2	2.21	0.41
1:B:851:ARG:O	1:B:852:MET:HB2	2.20	0.41
1:B:1059:PHE:HA	1:B:1060:PRO:HD3	1.80	0.41
1:C:832:LEU:HA	1:C:904:GLU:OE2	2.20	0.41
1:D:869:LEU:HD23	1:D:873:MET:HE2	2.01	0.41
1:A:1091:HIS:HE1	3:A:149:HOH:O	2.03	0.41
1:A:1099:LYS:HD3	1:A:1099:LYS:O	2.21	0.40
1:B:943:VAL:CG2	1:B:1114:VAL:HG11	2.51	0.40
1:C:854:TYR:N	1:C:854:TYR:CD1	2.87	0.40
1:C:1005:PHE:CE1	1:C:1009:LEU:HD11	2.57	0.40
1:D:1102:GLY:HA3	1:D:1109:PRO:CG	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1010:CYS:HB3	1:C:1017:VAL:HG12	2.03	0.40
1:D:1142:GLU:HA	1:D:1145:MET:CE	2.51	0.40
1:A:989:LYS:HA	1:A:992:ASP:OD2	2.21	0.40
1:C:1059:PHE:HA	1:C:1060:PRO:HD3	1.90	0.40
1:D:1019:LYS:HB3	1:D:1019:LYS:HZ3	1.85	0.40
1:D:1111:LYS:NZ	1:D:1111:LYS:HB3	2.36	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	304/340 (89%)	269 (88%)	29 (10%)	6 (2%)	7 14
1	B	319/340 (94%)	299 (94%)	14 (4%)	6 (2%)	8 15
1	C	270/340 (79%)	224 (83%)	40 (15%)	6 (2%)	6 12
1	D	296/340 (87%)	257 (87%)	31 (10%)	8 (3%)	5 8
All	All	1189/1360 (87%)	1049 (88%)	114 (10%)	26 (2%)	6 12

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	959	LEU
1	A	1014	HIS
1	A	1106	VAL
1	B	851	ARG
1	B	974	SER
1	B	975	ARG
1	B	1106	VAL
1	C	959	LEU
1	C	1106	VAL

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Mol	Chain	Res	Type
1	D	837	SER
1	D	893	LEU
1	D	1106	VAL
1	C	960	LEU
1	D	1060	PRO
1	A	998	GLN
1	B	849	SER
1	B	996	ALA
1	C	957	SER
1	D	851	ARG
1	D	1065	GLU
1	A	957	SER
1	A	1015	PRO
1	C	851	ARG
1	C	1010	CYS
1	D	929	PHE
1	D	1000	MET

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	285/309 (92%)	271 (95%)	14 (5%)	25 48
1	B	293/309 (95%)	278 (95%)	15 (5%)	24 46
1	C	258/309 (84%)	243 (94%)	15 (6%)	20 40
1	D	279/309 (90%)	265 (95%)	14 (5%)	24 47
All	All	1115/1236 (90%)	1057 (95%)	58 (5%)	23 46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	851	ARG
1	A	855	GLN
1	A	916	LEU
1	A	920	LEU

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Mol	Chain	Res	Type
1	A	950	LEU
1	A	1003	LEU
1	A	1005	PHE
1	A	1038	LEU
1	A	1079	ASP
1	A	1100	GLU
1	A	1110	LYS
1	A	1125	ARG
1	A	1138	ARG
1	A	1143	GLU
1	B	916	LEU
1	B	920	LEU
1	B	931	GLU
1	B	950	LEU
1	B	951	ARG
1	B	986	PHE
1	B	1003	LEU
1	B	1009	LEU
1	B	1018	LEU
1	B	1020	PHE
1	B	1038	LEU
1	B	1059	PHE
1	B	1087	LEU
1	B	1106	VAL
1	B	1110	LYS
1	C	843	LEU
1	C	866	GLU
1	C	916	LEU
1	C	920	LEU
1	C	931	GLU
1	C	956	PHE
1	C	962	LEU
1	C	1028	GLU
1	C	1038	LEU
1	C	1059	PHE
1	C	1068	LYS
1	C	1100	GLU
1	C	1110	LYS
1	C	1125	ARG
1	C	1147	ARG
1	D	893	LEU
1	D	916	LEU

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Mol	Chain	Res	Type
1	D	920	LEU
1	D	950	LEU
1	D	986	PHE
1	D	1009	LEU
1	D	1013	ASP
1	D	1032	ARG
1	D	1059	PHE
1	D	1065	GLU
1	D	1100	GLU
1	D	1120	ASP
1	D	1143	GLU
1	D	1149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	859	ASN
1	A	876	ASN
1	A	880	GLN
1	A	886	GLN
1	A	935	ASN
1	A	998	GLN
1	A	1012	ASN
1	A	1083	GLN
1	B	842	ASN
1	B	855	GLN
1	B	876	ASN
1	B	880	GLN
1	B	886	GLN
1	B	905	GLN
1	B	976	ASN
1	B	998	GLN
1	B	1057	GLN
1	B	1091	HIS
1	B	1123	ASN
1	B	1130	GLN
1	C	841	GLN
1	C	855	GLN
1	C	880	GLN
1	C	932	GLN
1	C	1037	ASN
1	C	1039	GLN

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Mol	Chain	Res	Type
1	C	1057	GLN
1	C	1085	ASN
1	C	1091	HIS
1	C	1123	ASN
1	C	1135	ASN
1	C	1136	GLN
1	D	841	GLN
1	D	842	ASN
1	D	876	ASN
1	D	886	GLN
1	D	932	GLN
1	D	955	ASN
1	D	1037	ASN
1	D	1058	ASN
1	D	1083	GLN
1	D	1126	ASN

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)

3 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	$\#\|Z\| > 2$
2	SO4	B	1164	-	4,4,4	0.39	0	6,6,6	0.28	0
2	SO4	C	1164	-	4,4,4	0.64	0	6,6,6	0.10	0
2	SO4	A	1164	-	4,4,4	0.55	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	308/340 (90%)	0.50	35 (11%) 5 3	23, 52, 116, 132	0
1	B	321/340 (94%)	0.29	17 (5%) 26 20	22, 43, 95, 129	0
1	C	278/340 (81%)	0.80	41 (14%) 2 1	41, 71, 127, 149	0
1	D	300/340 (88%)	1.24	70 (23%) 0 0	48, 85, 128, 152	0
All	All	1207/1360 (88%)	0.70	163 (13%) 3 1	22, 65, 121, 152	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	986	PHE	7.7
1	D	895	GLU	7.6
1	C	1145	MET	7.5
1	B	1150	LEU	7.2
1	C	1150	LEU	6.6
1	C	1014	HIS	6.0
1	D	837	SER	5.9
1	C	960	LEU	5.9
1	D	999	LYS	5.5
1	C	1106	VAL	5.4
1	D	1148	ALA	5.2
1	C	1147	ARG	5.2
1	D	1009	LEU	5.2
1	B	895	GLU	5.2
1	D	1043	ASP	5.0
1	A	829	VAL	4.9
1	D	997	ASP	4.9
1	D	1150	LEU	4.8
1	C	959	LEU	4.7
1	C	1108	ASP	4.6
1	D	1062	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	895	GLU	4.5
1	D	993	THR	4.4
1	D	1050	ALA	4.4
1	D	1013	ASP	4.3
1	B	892	GLU	4.3
1	B	1145	MET	4.3
1	D	841	GLN	4.3
1	C	1149	LYS	4.2
1	D	838	LYS	4.2
1	D	998	GLN	4.2
1	D	963	THR	4.2
1	C	1013	ASP	4.1
1	C	1006	LEU	4.1
1	A	960	LEU	4.1
1	D	995	SER	4.1
1	D	1039	GLN	4.1
1	C	1146	ARG	4.1
1	D	996	ALA	4.1
1	C	957	SER	4.0
1	C	1063	THR	4.0
1	A	1158	GLU	4.0
1	C	1010	CYS	3.9
1	D	1015	PRO	3.9
1	B	831	GLU	3.9
1	B	1148	ALA	3.8
1	D	992	ASP	3.8
1	C	1092	SER	3.8
1	A	1146	ARG	3.8
1	D	994	LYS	3.8
1	D	893	LEU	3.7
1	A	989	LYS	3.7
1	A	997	ASP	3.6
1	C	1009	LEU	3.6
1	A	992	ASP	3.5
1	D	852	MET	3.5
1	D	1102	GLY	3.5
1	C	1103	ASP	3.5
1	A	1022	ASP	3.5
1	D	1063	THR	3.5
1	D	1065	GLU	3.4
1	D	885	GLU	3.4
1	C	958	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	850	PHE	3.4
1	D	1071	GLU	3.4
1	D	1072	LYS	3.4
1	A	1013	ASP	3.3
1	D	961	GLU	3.3
1	B	975	ARG	3.3
1	C	1104	TYR	3.3
1	C	1144	LYS	3.3
1	A	1159	ARG	3.3
1	D	1054	ARG	3.3
1	A	954	GLU	3.2
1	D	840	ALA	3.2
1	A	958	SER	3.2
1	D	1001	THR	3.2
1	D	844	SER	3.1
1	C	1148	ALA	3.1
1	D	1111	LYS	3.1
1	B	885	GLU	3.1
1	B	1149	LYS	3.1
1	A	1108	ASP	3.1
1	D	985	SER	3.0
1	D	960	LEU	3.0
1	A	1106	VAL	3.0
1	D	1005	PHE	3.0
1	A	1019	LYS	3.0
1	D	892	GLU	3.0
1	D	894	LYS	3.0
1	D	883	GLU	2.9
1	D	1051	ASP	2.9
1	A	1111	LYS	2.9
1	A	988	CYS	2.9
1	A	1015	PRO	2.9
1	D	1061	ALA	2.9
1	D	877	LEU	2.9
1	D	845	ILE	2.9
1	D	1145	MET	2.9
1	D	988	CYS	2.8
1	D	831	GLU	2.8
1	D	1149	LYS	2.8
1	D	1112	LEU	2.8
1	C	1102	GLY	2.8
1	D	1064	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1012	ASN	2.7
1	A	1160	LEU	2.7
1	B	850	PHE	2.7
1	A	1021	PRO	2.6
1	A	1155	ALA	2.6
1	B	889	MET	2.6
1	D	1108	ASP	2.6
1	B	1147	ARG	2.6
1	B	894	LYS	2.5
1	D	1000	MET	2.5
1	D	1046	LYS	2.5
1	C	961	GLU	2.5
1	C	1064	ASP	2.5
1	A	957	SER	2.5
1	C	962	LEU	2.4
1	A	956	PHE	2.4
1	B	1146	ARG	2.4
1	D	957	SER	2.4
1	A	953	SER	2.4
1	C	1012	ASN	2.4
1	A	990	LEU	2.4
1	C	1061	ALA	2.4
1	A	1142	GLU	2.4
1	C	1107	PHE	2.4
1	A	1102	GLY	2.3
1	A	1016	GLU	2.3
1	C	1111	LYS	2.3
1	A	1018	LEU	2.3
1	C	1018	LEU	2.3
1	A	999	LYS	2.3
1	D	1103	ASP	2.3
1	B	844	SER	2.3
1	D	1058	ASN	2.3
1	D	1100	GLU	2.3
1	A	1157	LYS	2.3
1	D	1047	LYS	2.3
1	C	1142	GLU	2.2
1	D	1089	MET	2.2
1	C	1005	PHE	2.2
1	C	1017	VAL	2.2
1	C	1113	SER	2.2
1	C	1025	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1092	SER	2.2
1	D	1088	ARG	2.2
1	C	829	VAL	2.1
1	A	1151	ALA	2.1
1	B	838	LYS	2.1
1	D	989	LYS	2.1
1	B	1063	THR	2.1
1	D	1107	PHE	2.1
1	D	839	THR	2.1
1	A	1104	TYR	2.1
1	D	1085	ASN	2.1
1	A	1103	ASP	2.1
1	C	898	ASP	2.0
1	C	1003	LEU	2.0
1	C	1065	GLU	2.0
1	D	952	LYS	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^{th} 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^2)	Q<0.9
2	SO4	A	1164	5/5	0.94	0.21	86,86,87,87	0
2	SO4	C	1164	5/5	0.94	0.18	98,98,98,98	0
2	SO4	B	1164	5/5	0.97	0.14	68,71,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.