



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:23 AM UTC

PDB ID : 1V9D / pdb_00001v9d
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

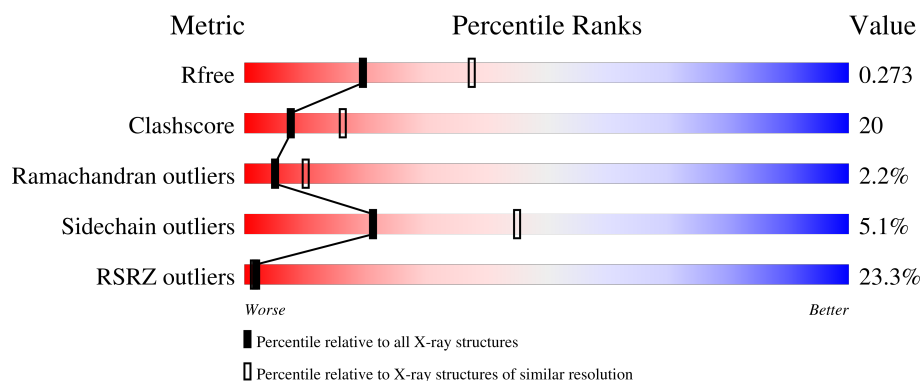
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	340	16% 51% 34% 5% 9%
1	B	340	10% 64% 28% • 6%
1	C	340	21% 46% 31% • 18%
1	D	340	36% 49% 35% • 12%

2 Entry composition

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 (CCD ID: SO4) (formula: O₄S).



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

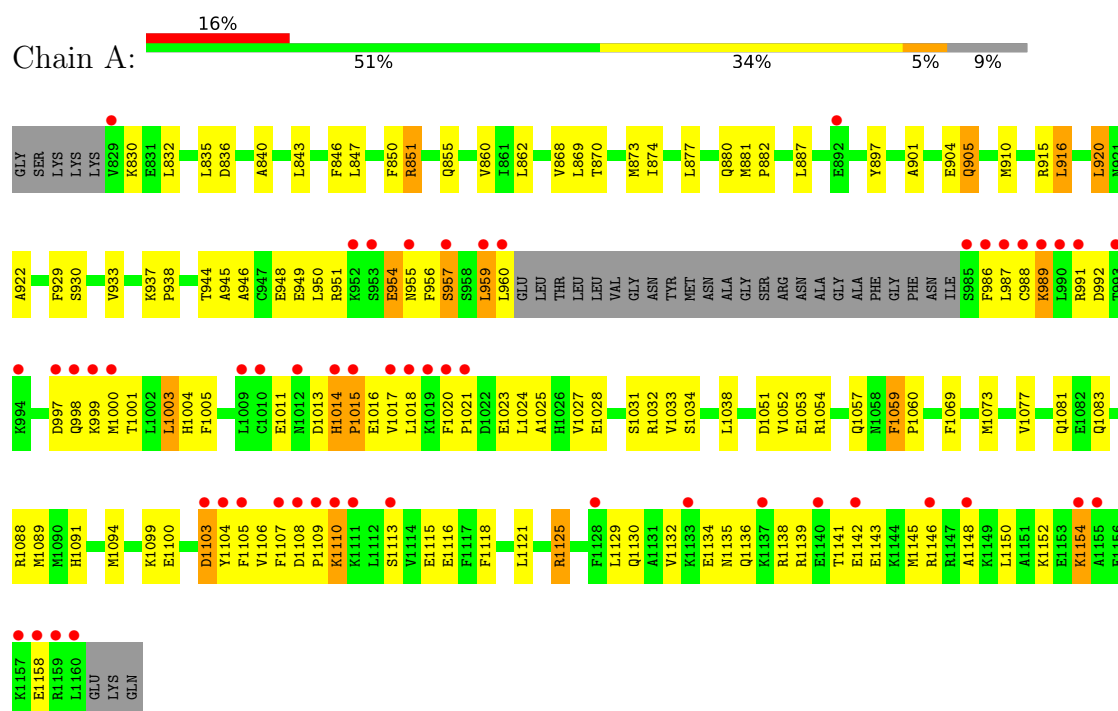
- Molecule 3 is water.

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

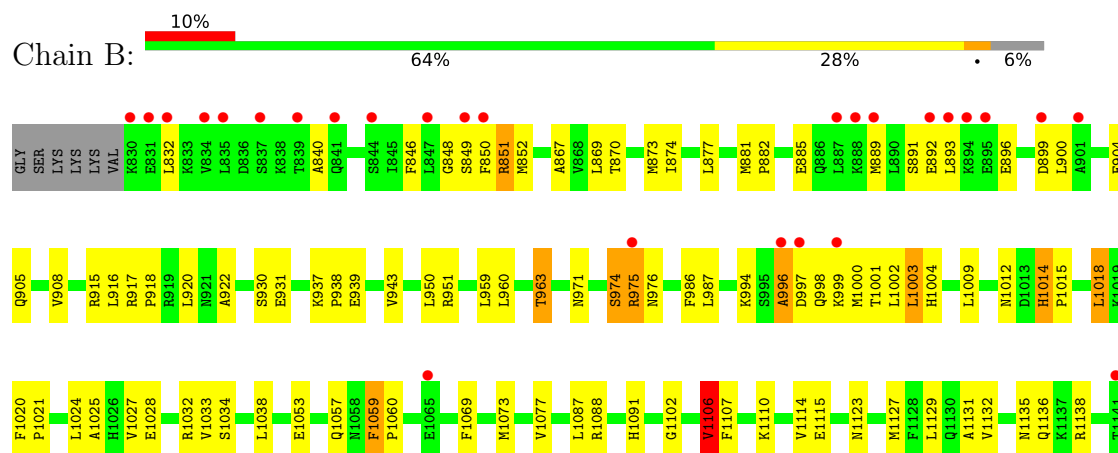
3 Residue-property plots [i](#)

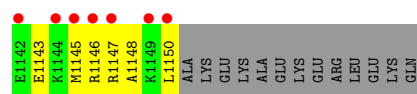
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

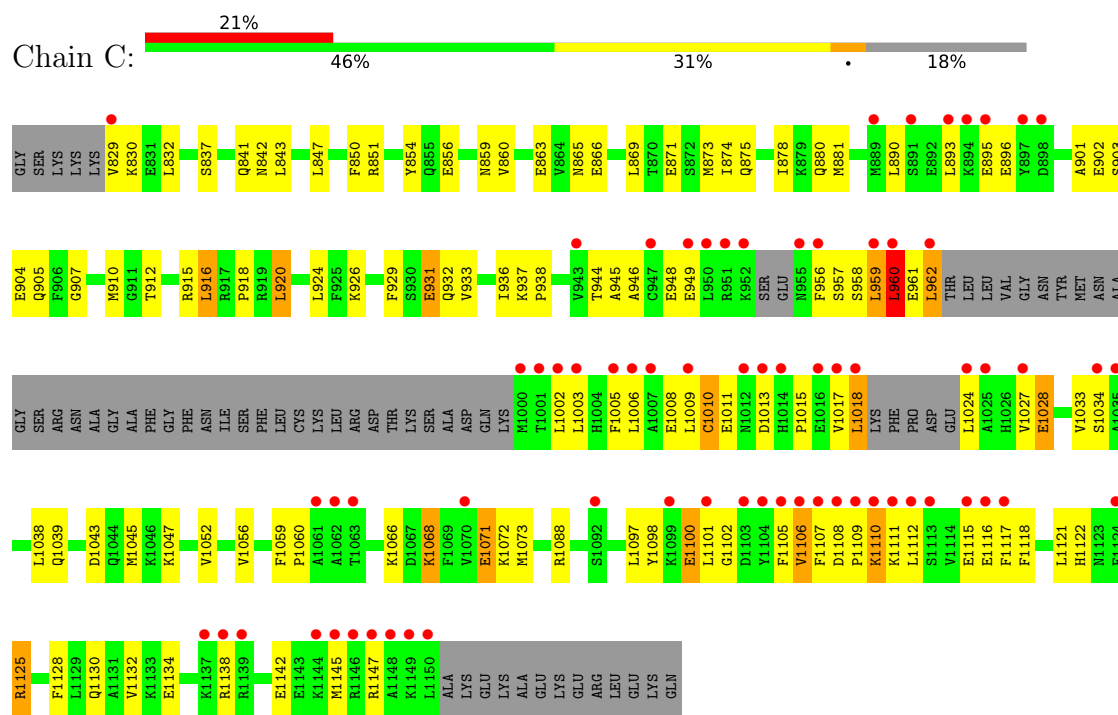


• Molecule 1: Diaphanous protein homolog 1

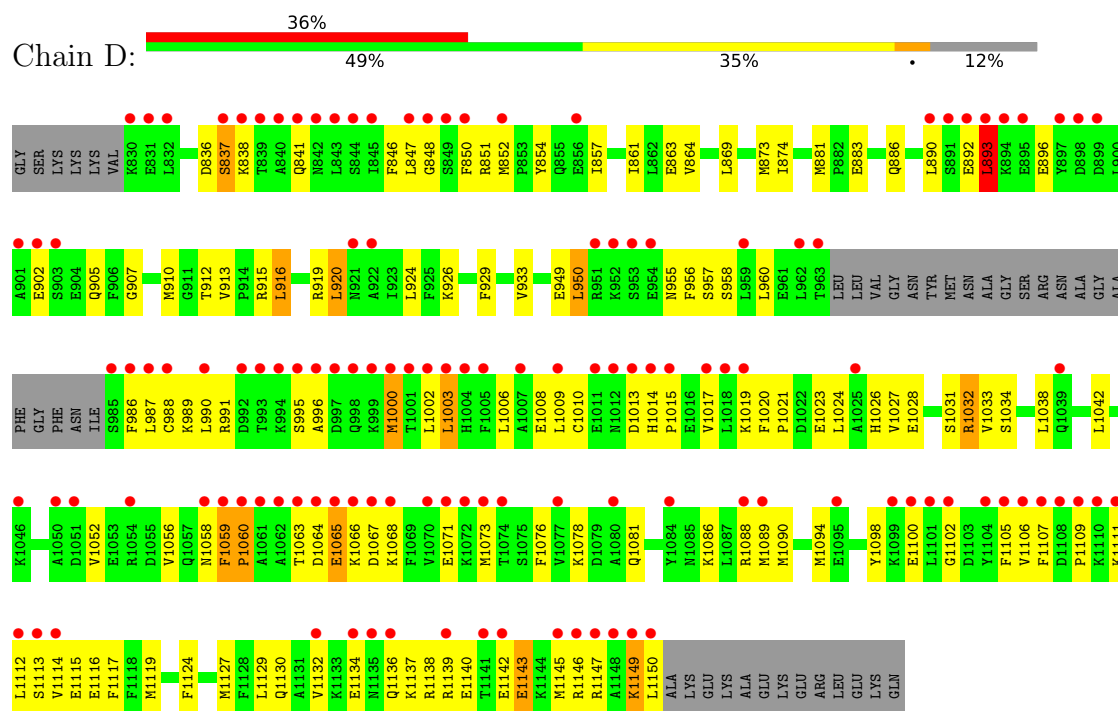




- Molecule 1: Diaphanous protein homolog 1



- Molecule 1: Diaphanous protein homolog 1



4 Data and refinement statistics

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) 85.5 (29.12-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.47 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.267 (Not available) , 0.273	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)	0.32 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

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	0.46	0/2560	0.91	10/3427 (0.3%)
1	B	0.48	0/2651	0.93	14/3555 (0.4%)
1	C	0.36	0/2310	0.84	4/3094 (0.1%)
1	D	0.33	0/2494	0.88	4/3342 (0.1%)
All	All	0.41	0/10015	0.89	32/13418 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	913	VAL	N-CA-C	8.83	115.60	107.56
1	A	929	PHE	N-CA-C	7.89	120.65	111.02
1	B	997	ASP	N-CA-C	-6.59	100.53	110.28
1	B	1025	ALA	N-CA-C	6.39	119.93	111.75
1	B	905	GLN	N-CA-C	-6.07	104.74	111.36
1	B	867	ALA	N-CA-C	-5.97	105.99	113.28
1	A	933	VAL	N-CA-C	-5.97	104.50	111.00
1	B	939	GLU	N-CA-C	-5.88	104.78	111.07
1	C	850	PHE	N-CA-C	-5.84	104.99	111.36
1	D	905	GLN	N-CA-C	-5.82	105.01	111.36
1	C	1100	GLU	N-CA-C	-5.78	105.33	112.38
1	B	1148	ALA	N-CA-C	-5.68	106.31	113.18
1	C	929	PHE	N-CA-C	5.67	120.67	111.37
1	D	933	VAL	N-CA-C	-5.65	104.84	111.00
1	B	1059	PHE	CA-C-N	5.52	125.28	119.76
1	B	1059	PHE	C-N-CA	5.52	125.28	119.76
1	A	1059	PHE	N-CA-C	5.50	116.59	109.72
1	B	1069	PHE	N-CA-C	5.36	117.56	111.02
1	D	1063	THR	N-CA-C	-5.35	106.78	113.15
1	A	1025	ALA	N-CA-C	5.23	117.66	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	954	GLU	N-CA-C	-5.18	105.81	111.82
1	A	1052	VAL	N-CA-C	-5.17	105.46	110.42
1	A	1089	MET	N-CA-C	-5.15	104.74	111.02
1	A	905	GLN	N-CA-C	-5.10	105.80	111.36
1	C	933	VAL	N-CA-C	-5.08	105.58	110.72
1	B	1145	MET	N-CA-C	-5.07	105.83	111.36
1	A	868	VAL	CB-CA-C	-5.06	106.55	111.05
1	A	1154	LYS	N-CA-C	-5.04	105.92	111.71
1	B	1001	THR	N-CA-C	-5.03	103.08	110.52
1	B	1014	HIS	CA-C-N	5.02	124.46	119.24
1	B	1014	HIS	C-N-CA	5.02	124.46	119.24
1	B	1012	ASN	N-CA-C	5.01	116.55	111.14

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	115	0
1	B	2611	0	2627	70	0
1	C	2279	0	2303	108	0
1	D	2458	0	2479	108	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	4	0
3	C	18	0	0	5	0
3	D	8	0	0	0	0
All	All	10079	0	9964	398	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 20.

All (398) 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:B:869:LEU:HD23	1:B:873:MET:HE2	1.48	0.96
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:922:ALA:HB1	1:A:1073:MET:HE2	1.51	0.91
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:869:LEU:HD23	1:A:873:MET:HE2	1.58	0.84
1:A:850:PHE:HB3	3:A:168:HOH:O	1.79	0.82
1:C:869:LEU:HD23	1:C:873:MET:HE2	1.62	0.80
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:D:991:ARG:HB2	1:D:1003:LEU:HD12	1.67	0.75
1:D:869:LEU:HD23	1:D:873:MET:HE2	1.68	0.74
1:D:1032:ARG:HG2	1:D:1032:ARG:HH11	1.51	0.74
1:C:910:MET:HE2	1:C:910:MET:HA	1.69	0.74
1:C:1013:ASP:C	1:C:1015:PRO:HD3	2.13	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:B:852:MET:HE2	3:B:153:HOH:O	1.89	0.72
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:C:961:GLU:CD	1:C:961:GLU:H	1.98	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: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
1:C:1097:LEU:O	1:C:1101:LEU:HD23	1.94	0.68
1:B:892:GLU:C	1:B:893:LEU:HD12	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:881:MET:HE2	1:A:887:LEU:HD11	1.75	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:C:1034:SER:HA	1:C:1115:GLU:CD	2.19	0.66
1:A:1031:SER:HA	3:A:195:HOH:O	1.93	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:1147:ARG:C	1:C:1147:ARG:HD3	2.22	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: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:B:848:GLY:C	1:B:850:PHE:H	2.05	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: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:B:869:LEU:CD2	1:B:873:MET:HE2	2.29	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
1:D:1149:LYS:HD2	1:D:1149:LYS:C	2.26	0.60
1:A:1000:MET:HG2	1:A:1001:THR:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1011:GLU:CD	1:A:1139:ARG:HH22	2.09	0.60
1:B:1135:ASN:HA	1:B:1138:ARG:NH1	2.16	0.60
1:D:1019:LYS:HB3	1:D:1019:LYS:NZ	2.17	0.60
1:D:1014:HIS:O	1:D:1017:VAL:HG22	2.01	0.59
1:D:1089:MET:HE2	1:D:1089:MET:HA	1.82	0.59
1:A:916:LEU:HD22	1:A:920:LEU:HD22	1.84	0.59
1:C:869:LEU:HD23	1:C:873:MET:CE	2.30	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:D:1038:LEU:HD23	1:D:1094:MET:HE1	1.84	0.59
1:A:944:THR:O	1:A:948:GLU:HG3	2.02	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:B:999:LYS:O	1:B:999:LYS:HG2	2.03	0.58
1:D:1028:GLU:HG2	1:D:1032:ARG:HH21	1.69	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:D:881:MET:HE3	1:D:916:LEU:HD21	1.86	0.57
1:A:1033:VAL:HG12	1:A:1034:SER:N	2.19	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:D:874:ILE:HG21	1:D:924:LEU:HB2	1.86	0.56
1:D:1142:GLU:HA	1:D:1145:MET:HE3	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:LEU:C	1:C:1011:GLU:H	2.13	0.56
1:B:885:GLU:H	1:B:885:GLU:CD	2.14	0.56
1:C:960:LEU:C	1:C:960:LEU:HD23	2.31	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:C:926:LYS:HB2	1:C:1073:MET:HE1	1.89	0.55
1:D:1032:ARG:HG2	1:D:1032:ARG:NH1	2.22	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:D:869:LEU:CD2	1:D:873:MET:HE2	2.36	0.55
1:C:1024:LEU:N	3:C:127:HOH:O	2.39	0.55
1:D:988:CYS:HB3	1:D:1127:MET:HE1	1.88	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:D:926:LYS:HD2	1:D:1073:MET:HE1	1.91	0.53
1:A:1088:ARG:HH11	1:A:1088:ARG:HG3	1.74	0.53
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:A:1099:LYS:C	1:A:1099:LYS:HD3	2.35	0.52
1:C:1028:GLU:HG2	1:C:1122:HIS:CE1	2.45	0.52
1:B:869:LEU:HD23	1:B:873:MET:CE	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1056:VAL:C	1:D:1058:ASN:H	2.18	0.52
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:848:GLY:C	1:B:850:PHE:N	2.68	0.51
1:B:1033:VAL:HG12	1:B:1034:SER:N	2.25	0.51
1:A:869:LEU:CD2	1:A:873:MET:HE2	2.37	0.51
1:D:1149:LYS:HE2	1:D:1150:LEU:CD1	2.40	0.51
1:A:997:ASP:C	1:A:999:LYS:H	2.19	0.51
1:D:1000:MET:HE1	1:D:1008:GLU:OE2	2.10	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:1067:ASP:C	1:D:1068:LYS:HD2	2.36	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:C:1147:ARG:C	1:C:1147:ARG:CD	2.83	0.51
1:A:997:ASP:C	1:A:999:LYS:N	2.68	0.50
1:D:1010:CYS:HA	1:D:1014:HIS:HB2	1.93	0.50
1:C:1011:GLU:C	1:C:1015:PRO:HG3	2.37	0.50
1:C:944:THR:O	1:C:948:GLU:HG3	2.11	0.50
1:D:1065:GLU:CD	1:D:1065:GLU:H	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:1064:ASP:C	1:D:1066:LYS:H	2.21	0.48
1:A:937:LYS:HB3	1:A:938:PRO:HD3	1.95	0.48
1:D:1138:ARG:C	1:D:1140:GLU:H	2.21	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: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:B:1020:PHE:CD1	1:B:1020:PHE:C	2.92	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:A:1027:VAL:HG11	1:A:1121:LEU:HD12	1.96	0.47
1:A:1108:ASP:CG	1:A:1110:LYS:HE3	2.40	0.47
1:C:1138:ARG:NH1	3:C:182:HOH:O	2.47	0.47
1:D:1019:LYS:HB3	1:D:1019:LYS:HZ2	1.79	0.47
1:A:846:PHE:CG	1:A:880:GLN:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:VAL:O	1:C:830:LYS:HB2	2.14	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:1109:PRO:C	1:C:1110:LYS:HD3	2.40	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:B:1138:ARG:HH11	1:B:1138:ARG:CB	2.28	0.46
1:D:1033:VAL:HG12	1:D:1034:SER:N	2.30	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:1004:HIS:HB3	1:A:1135:ASN:OD1	2.15	0.46
1:A:1141:THR:HG22	1:A:1145:MET:HE2	1.98	0.46
1:D:955:ASN:HD22	1:D:1023:GLU:CD	2.24	0.46
1:C:830:LYS:HD3	1:C:901:ALA:HA	1.98	0.46
1:C:1142:GLU:HA	1:C:1142:GLU:OE2	2.16	0.46
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:D:910:MET:HA	1:D:910:MET:HE2	1.97	0.45
1:C:1112:LEU:HD12	1:C:1116:GLU:OE1	2.17	0.45
1:D:987:LEU:C	1:D:989:LYS:H	2.25	0.45
1:A:910:MET:HE3	1:A:916:LEU:HD11	1.98	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:B:922:ALA:CB	1:B:1073:MET:HE3	2.47	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:D:1056:VAL:C	1:D:1058:ASN:N	2.73	0.45
1:A:881:MET:HE1	1:A:887:LEU:HD11	1.98	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:ASP:O	1:A:1014:HIS:HB2	2.17	0.44
1:B:959:LEU:HD13	1:B:959:LEU:C	2.42	0.44
1:B:960:LEU:O	1:B:963:THR:HB	2.18	0.44
1:B:986:PHE:C	1:B:986:PHE:CD2	2.95	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:A:1103:ASP:C	1:A:1105:PHE:H	2.25	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
1:A:881:MET:HE3	1:A:882:PRO:HD2	1.99	0.44
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:1105:PHE:O	1:C:1106:VAL:C	2.61	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:A:1000:MET:HE3	1:A:1005:PHE:N	2.33	0.43
1:A:1014:HIS:C	1:A:1016:GLU:H	2.26	0.43
1:B:1020:PHE:N	1:B:1021:PRO:CD	2.81	0.43
1:C:910:MET:HE2	1:C:910:MET:CA	2.45	0.43
1:C:1002:LEU:HD23	1:C:1002:LEU:C	2.44	0.43
1:B:1088:ARG:HD3	3:B:112:HOH:O	2.18	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:A:986:PHE:C	1:A:988:CYS:N	2.73	0.43
1:B:904:GLU:O	1:B:908:VAL:HG23	2.19	0.43
1:C:915:ARG:O	1:C:916:LEU:C	2.61	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:D:1038:LEU:CD2	1:D:1094:MET:HE1	2.49	0.43
1:C:880:GLN:NE2	3:C:174:HOH:O	2.50	0.43
1:D:995:SER:O	1:D:996:ALA:C	2.61	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:D:1013:ASP:C	1:D:1014:HIS:ND1	2.77	0.43
1:A:1018:LEU:HD23	1:A:1018:LEU:C	2.44	0.43
1:A:1021:PRO:HG2	1:A:1129:LEU:CD2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1106:VAL:O	1:C:1106:VAL:HG13	2.18	0.43
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:A:1103:ASP:C	1:A:1105:PHE:N	2.77	0.42
1:B:848:GLY:O	1:B:850:PHE:N	2.52	0.42
1:B:922:ALA:HB1	1:B:1073:MET:HE3	2.00	0.42
1:D:916:LEU:O	1:D:919:ARG:HB3	2.19	0.42
1:D:1006:LEU:C	1:D:1006:LEU:HD23	2.44	0.42
1:A:959:LEU:O	1:A:960:LEU:HG	2.19	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
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:956:PHE:O	1:A:957:SER:C	2.62	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:D:836:ASP:O	1:D:837:SER:C	2.63	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: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: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:B:1107:PHE:CD1	1:B:1107:PHE:C	2.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:LEU:HB3	1:B:1027:VAL:HG21	2.01	0.41
1:D:848:GLY:C	1:D:850:PHE:H	2.26	0.41
1:D:1017:VAL:C	1:D:1019:LYS:H	2.29	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: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:B:889:MET:C	1:B:891:SER:H	2.29	0.41
1:C:832:LEU:HA	1:C:904:GLU:OE2	2.20	0.41
1:C:910:MET:C	1:C:912:THR:H	2.29	0.41
1:C:1009:LEU:C	1:C:1011:GLU:N	2.79	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:932:GLN:HE21	1:C:1045:MET:HE2	1.86	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
1:C:1010:CYS:HB3	1:C:1017:VAL:HG12	2.03	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: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%)	6	12
1	B	319/340 (94%)	299 (94%)	14 (4%)	6 (2%)	6	13
1	C	270/340 (79%)	224 (83%)	40 (15%)	6 (2%)	5	10
1	D	296/340 (87%)	257 (87%)	31 (10%)	8 (3%)	4	7
All	All	1189/1360 (87%)	1049 (88%)	114 (10%)	26 (2%)	5	10

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
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 ⓘ

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%)	269 (94%)	16 (6%)	19	40
1	B	293/309 (95%)	279 (95%)	14 (5%)	23	47
1	C	258/309 (84%)	242 (94%)	16 (6%)	16	36
1	D	279/309 (90%)	268 (96%)	11 (4%)	28	55
All	All	1115/1236 (90%)	1058 (95%)	57 (5%)	21	45

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	830	LYS
1	A	851	ARG
1	A	855	GLN
1	A	860	VAL
1	A	916	LEU
1	A	920	LEU
1	A	950	LEU
1	A	989	LYS
1	A	1003	LEU
1	A	1038	LEU
1	A	1100	GLU
1	A	1103	ASP
1	A	1110	LYS
1	A	1125	ARG
1	A	1143	GLU
1	A	1150	LEU
1	B	916	LEU
1	B	920	LEU
1	B	931	GLU
1	B	950	LEU
1	B	951	ARG
1	B	963	THR
1	B	1003	LEU
1	B	1009	LEU
1	B	1018	LEU
1	B	1038	LEU
1	B	1077	VAL
1	B	1087	LEU
1	B	1106	VAL
1	B	1110	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	866	GLU
1	C	893	LEU
1	C	916	LEU
1	C	920	LEU
1	C	931	GLU
1	C	956	PHE
1	C	960	LEU
1	C	962	LEU
1	C	1018	LEU
1	C	1028	GLU
1	C	1038	LEU
1	C	1068	LYS
1	C	1071	GLU
1	C	1100	GLU
1	C	1110	LYS
1	C	1125	ARG
1	D	893	LEU
1	D	916	LEU
1	D	920	LEU
1	D	950	LEU
1	D	1003	LEU
1	D	1009	LEU
1	D	1032	ARG
1	D	1059	PHE
1	D	1100	GLU
1	D	1143	GLU
1	D	1149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	905	GLN
1	A	932	GLN
1	A	935	ASN
1	A	998	GLN
1	A	1012	ASN
1	A	1048	GLN
1	A	1083	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1091	HIS
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	1057	GLN
1	B	1091	HIS
1	B	1123	ASN
1	C	841	GLN
1	C	855	GLN
1	C	880	GLN
1	C	932	GLN
1	C	1037	ASN
1	C	1039	GLN
1	C	1048	GLN
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	998	GLN
1	D	1037	ASN
1	D	1058	ASN
1	D	1083	GLN
1	D	1126	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.48	0	6,6,6	0.28	0
2	SO4	C	1164	-	4,4,4	0.71	0	6,6,6	0.12	0
2	SO4	A	1164	-	4,4,4	0.63	0	6,6,6	0.13	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 [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, 95th 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%)	0.81	53 (17%) 4 3	23, 52, 116, 132	0
1	B	321/340 (94%)	0.40	34 (10%) 11 9	22, 43, 95, 129	0
1	C	278/340 (81%)	1.34	70 (25%) 1 1	41, 71, 127, 149	0
1	D	300/340 (88%)	1.90	124 (41%) 0 0	48, 85, 128, 152	0
All	All	1207/1360 (88%)	1.10	281 (23%) 2 1	22, 65, 121, 152	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1150	LEU	7.5
1	C	1018	LEU	6.8
1	A	952	LYS	6.7
1	C	1150	LEU	6.3
1	A	1018	LEU	6.3
1	D	1107	PHE	6.3
1	B	1149	LYS	6.0
1	D	1015	PRO	5.8
1	C	1013	ASP	5.7
1	C	1148	ALA	5.6
1	A	985	SER	5.5
1	D	1009	LEU	5.5
1	D	985	SER	5.1
1	C	895	GLU	5.1
1	B	1150	LEU	5.0
1	D	1005	PHE	4.9
1	A	998	GLN	4.9
1	D	954	GLU	4.8
1	D	1145	MET	4.6
1	A	960	LEU	4.6
1	C	1014	HIS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1101	LEU	4.5
1	D	1112	LEU	4.5
1	B	893	LEU	4.5
1	B	997	ASP	4.5
1	A	999	LYS	4.4
1	D	953	SER	4.4
1	D	1062	ALA	4.4
1	D	986	PHE	4.4
1	A	1160	LEU	4.4
1	D	894	LYS	4.4
1	D	1068	LYS	4.4
1	A	990	LEU	4.3
1	D	993	THR	4.3
1	D	997	ASP	4.3
1	B	894	LYS	4.3
1	D	1001	THR	4.2
1	D	994	LYS	4.2
1	C	962	LEU	4.2
1	D	1106	VAL	4.2
1	D	1002	LEU	4.2
1	C	1112	LEU	4.1
1	D	952	LYS	4.1
1	D	1149	LYS	4.1
1	C	1106	VAL	4.0
1	C	1024	LEU	4.0
1	C	1144	LYS	4.0
1	D	988	CYS	4.0
1	D	999	LYS	4.0
1	C	960	LEU	3.9
1	A	986	PHE	3.9
1	C	1105	PHE	3.9
1	A	1019	LYS	3.9
1	C	1107	PHE	3.9
1	D	847	LEU	3.9
1	D	1003	LEU	3.9
1	C	1035	ALA	3.8
1	A	994	LYS	3.8
1	B	999	LYS	3.8
1	D	895	GLU	3.8
1	A	988	CYS	3.8
1	C	1147	ARG	3.8
1	D	830	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1145	MET	3.7
1	D	963	THR	3.7
1	D	996	ALA	3.7
1	A	1017	VAL	3.6
1	A	829	VAL	3.6
1	D	1109	PRO	3.6
1	D	1072	LYS	3.5
1	C	1063	THR	3.5
1	D	1017	VAL	3.5
1	D	1113	SER	3.5
1	A	1108	ASP	3.5
1	D	1000	MET	3.4
1	D	1070	VAL	3.4
1	D	893	LEU	3.4
1	A	1015	PRO	3.4
1	D	1100	GLU	3.4
1	C	952	LYS	3.3
1	D	1063	THR	3.3
1	A	991	ARG	3.3
1	C	951	ARG	3.3
1	A	1155	ALA	3.3
1	A	997	ASP	3.3
1	C	1016	GLU	3.3
1	D	890	LEU	3.3
1	D	902	GLU	3.3
1	B	889	MET	3.3
1	D	1108	ASP	3.3
1	B	895	GLU	3.3
1	A	1137	LYS	3.3
1	D	1088	ARG	3.2
1	A	993	THR	3.2
1	D	995	SER	3.2
1	C	1111	LYS	3.2
1	D	1013	ASP	3.2
1	C	1002	LEU	3.2
1	D	831	GLU	3.2
1	D	992	ASP	3.1
1	A	1021	PRO	3.1
1	D	901	ALA	3.1
1	D	844	SER	3.1
1	A	1105	PHE	3.1
1	D	1146	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	852	MET	3.1
1	B	849	SER	3.1
1	A	959	LEU	3.1
1	C	955	ASN	3.1
1	D	843	LEU	3.1
1	B	996	ALA	3.1
1	C	1146	ARG	3.1
1	C	956	PHE	3.1
1	A	1104	TYR	3.0
1	C	893	LEU	3.0
1	A	1157	LYS	3.0
1	A	953	SER	3.0
1	A	1110	LYS	3.0
1	D	1061	ALA	3.0
1	C	1092	SER	3.0
1	A	1159	ARG	3.0
1	D	892	GLU	3.0
1	A	1109	PRO	3.0
1	C	1139	ARG	3.0
1	C	1116	GLU	2.9
1	A	957	SER	2.9
1	D	1110	LYS	2.9
1	D	1148	ALA	2.9
1	A	1113	SER	2.9
1	D	841	GLN	2.9
1	C	1104	TYR	2.9
1	C	1108	ASP	2.9
1	B	831	GLU	2.9
1	A	1146	ARG	2.9
1	A	1103	ASP	2.9
1	C	1005	PHE	2.9
1	D	1114	VAL	2.8
1	D	1071	GLU	2.8
1	C	1012	ASN	2.8
1	C	1003	LEU	2.8
1	C	1009	LEU	2.8
1	D	839	THR	2.8
1	D	1077	VAL	2.8
1	D	1018	LEU	2.8
1	B	899	ASP	2.8
1	D	1105	PHE	2.8
1	D	951	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1019	LYS	2.7
1	D	921	ASN	2.7
1	C	1062	ALA	2.7
1	D	1051	ASP	2.7
1	B	830	LYS	2.7
1	C	1137	LYS	2.7
1	A	1107	PHE	2.7
1	B	1142	GLU	2.7
1	C	1149	LYS	2.7
1	D	850	PHE	2.7
1	D	1099	LYS	2.7
1	C	1006	LEU	2.6
1	D	1147	ARG	2.6
1	D	1111	LYS	2.6
1	B	901	ALA	2.6
1	D	897	TYR	2.6
1	D	838	LYS	2.6
1	D	848	GLY	2.6
1	C	1017	VAL	2.6
1	A	1020	PHE	2.6
1	C	1124	PHE	2.6
1	D	1139	ARG	2.6
1	A	1014	HIS	2.6
1	B	1141	THR	2.5
1	C	1034	SER	2.5
1	D	987	LEU	2.5
1	B	1146	ARG	2.5
1	C	1113	SER	2.5
1	D	837	SER	2.5
1	B	832	LEU	2.5
1	B	839	THR	2.5
1	C	1103	ASP	2.5
1	C	1000	MET	2.5
1	D	1136	GLN	2.5
1	C	1101	LEU	2.5
1	D	959	LEU	2.5
1	D	1064	ASP	2.5
1	A	1140	GLU	2.5
1	B	892	GLU	2.5
1	D	1080	ALA	2.5
1	A	987	LEU	2.4
1	D	1134	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	894	LYS	2.4
1	D	840	ALA	2.4
1	B	837	SER	2.4
1	B	844	SER	2.4
1	D	898	ASP	2.4
1	A	1154	LYS	2.4
1	C	1099	LYS	2.4
1	D	845	ILE	2.4
1	A	1012	ASN	2.4
1	D	1058	ASN	2.4
1	C	829	VAL	2.4
1	A	955	ASN	2.4
1	D	1060	PRO	2.4
1	D	1039	GLN	2.4
1	C	1061	ALA	2.4
1	D	962	LEU	2.3
1	D	1084	TYR	2.3
1	A	989	LYS	2.3
1	D	1067	ASP	2.3
1	C	943	VAL	2.3
1	C	1117	PHE	2.3
1	C	959	LEU	2.3
1	A	1111	LYS	2.3
1	B	975	ARG	2.3
1	A	1010	CYS	2.3
1	D	990	LEU	2.3
1	D	1011	GLU	2.3
1	C	891	SER	2.3
1	D	998	GLN	2.3
1	A	1009	LEU	2.3
1	B	847	LEU	2.3
1	A	1148	ALA	2.3
1	C	897	TYR	2.3
1	A	1142	GLU	2.3
1	A	1158	GLU	2.3
1	D	842	ASN	2.3
1	C	898	ASP	2.3
1	A	1133	LYS	2.2
1	D	856	GLU	2.2
1	D	1054	ARG	2.2
1	C	1109	PRO	2.2
1	D	1132	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	888	LYS	2.2
1	B	1144	LYS	2.2
1	C	1001	THR	2.2
1	B	1147	ARG	2.2
1	D	1012	ASN	2.2
1	C	1007	ALA	2.2
1	C	1138	ARG	2.2
1	D	849	SER	2.2
1	C	1025	ALA	2.2
1	A	892	GLU	2.2
1	C	1110	LYS	2.2
1	B	887	LEU	2.2
1	D	1102	GLY	2.2
1	D	903	SER	2.2
1	B	1065	GLU	2.1
1	C	1115	GLU	2.1
1	D	1142	GLU	2.1
1	B	835	LEU	2.1
1	C	950	LEU	2.1
1	B	850	PHE	2.1
1	D	1025	ALA	2.1
1	C	949	GLU	2.1
1	D	1046	LYS	2.1
1	B	841	GLN	2.1
1	A	1128	PHE	2.1
1	D	922	ALA	2.1
1	D	1065	GLU	2.1
1	A	1000	MET	2.1
1	D	832	LEU	2.1
1	C	947	CYS	2.1
1	D	1014	HIS	2.1
1	C	1027	VAL	2.1
1	C	1070	VAL	2.1
1	D	891	SER	2.1
1	D	1050	ALA	2.1
1	D	1066	LYS	2.1
1	D	1074	THR	2.1
1	B	1145	MET	2.1
1	D	1073	MET	2.1
1	B	834	VAL	2.1
1	D	1095	GLU	2.0
1	D	1141	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	889	MET	2.0
1	D	1089	MET	2.0
1	D	1004	HIS	2.0
1	D	1135	ASN	2.0
1	D	1104	TYR	2.0
1	D	1059	PHE	2.0
1	D	899	ASP	2.0
1	D	1007	ALA	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 oligosaccharides 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, 95th 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	C	1164	5/5	0.82	0.18	98,98,98,98	0
2	SO4	A	1164	5/5	0.93	0.16	86,86,87,87	0
2	SO4	B	1164	5/5	0.94	0.10	68,71,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.