Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:34 AM GMT

PDB ID	:	2HQC
Title	:	Conformation of the AcrB Multidrug Efflux Pump in Mutants of the Putative Proton Relay Pathway
Authors	:	Su, C.-C.; Li, M.; Gu, R.; Takatsuka, Y.; McDermott, G.; Nikaido, H.; Yu, E.W.
Deposited on	:	2006-07-18
Resolution	:	3.56 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

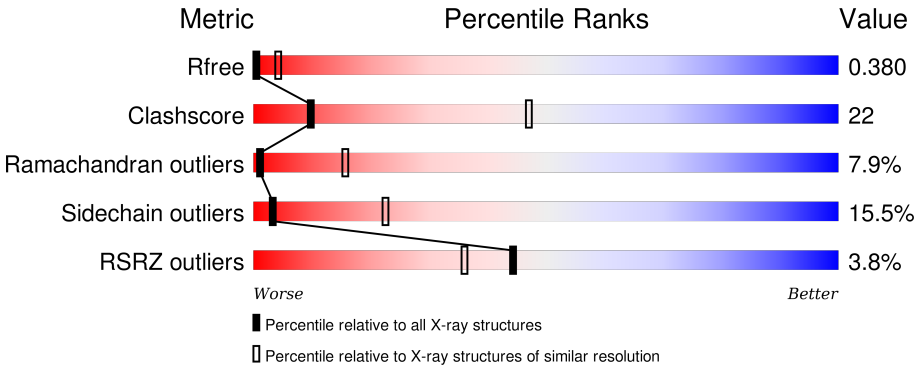
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.56 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1053	4% 51% 35% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7718 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	0	0	0
			7718	4964	1276	1435	43			

There are 5 discrepancies between the modelled and reference sequences:

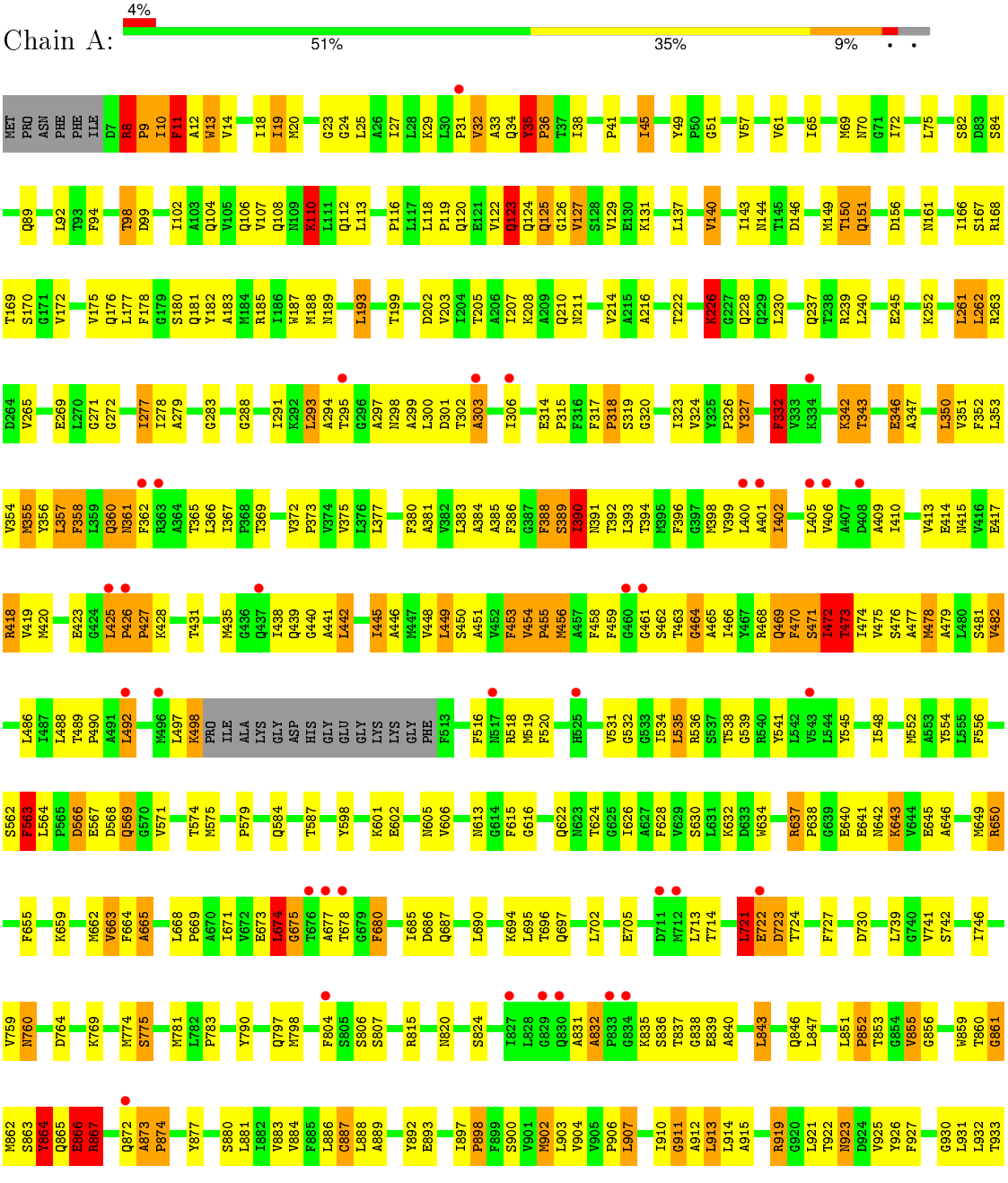
Chain	Residue	Modelled	Actual	Comment	Reference
A	407	ALA	ASP	ENGINEERED	UNP P31224
A	1050	HIS	-	CLONING ARTIFACT	UNP P31224
A	1051	HIS	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	CLONING ARTIFACT	UNP P31224
A	1053	HIS	-	CLONING ARTIFACT	UNP P31224

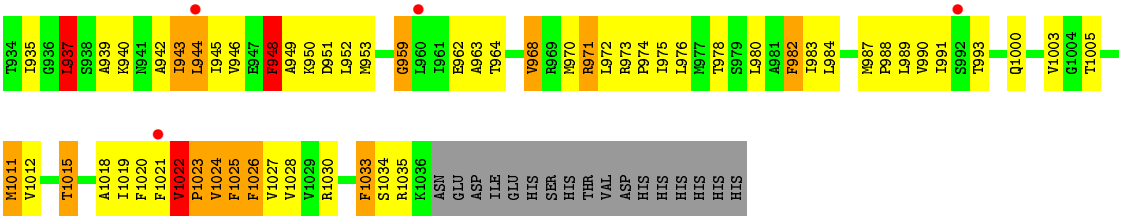
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Acriflavine resistance protein B

Chain A:




T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953 G959 L960 I961 E962 A963 T964 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 M987 P988 L989 V990 I991 S992 T993 Q1000 V1003 G1004 T1005
M1011 V1012 T1015 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 F1033 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	145.40Å 145.40Å 514.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.56 46.80 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-3.56) 95.8 (46.80-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.271 , 0.294 0.384 , 0.380	Depositor DCC
R_{free} test set	1274 reflections (5.53%)	DCC
Wilson B-factor (Å^2)	96.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	0 of 33665 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.83	26/7861 (0.3%)	0.71	12/10676 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	866	GLU	CD-OE2	21.22	1.49	1.25
1	A	110	LYS	CE-NZ	8.45	1.70	1.49
1	A	856	GLY	C-O	8.21	1.36	1.23
1	A	388	PHE	C-O	-7.89	1.08	1.23
1	A	332	PHE	CG-CD1	7.84	1.50	1.38
1	A	482	VAL	CB-CG2	7.44	1.68	1.52
1	A	705	GLU	CD-OE1	6.97	1.33	1.25
1	A	948	PHE	CG-CD1	6.90	1.49	1.38
1	A	418	ARG	CZ-NH1	6.83	1.42	1.33
1	A	332	PHE	CE2-CZ	6.76	1.50	1.37
1	A	673	GLU	C-O	6.20	1.35	1.23
1	A	705	GLU	CD-OE2	5.93	1.32	1.25
1	A	948	PHE	CE2-CZ	5.87	1.48	1.37
1	A	628	PHE	CG-CD2	5.86	1.47	1.38
1	A	123	GLN	CG-CD	5.66	1.64	1.51
1	A	948	PHE	CG-CD2	5.63	1.47	1.38
1	A	628	PHE	CG-CD1	5.55	1.47	1.38
1	A	866	GLU	CG-CD	5.50	1.60	1.51
1	A	628	PHE	CE1-CZ	5.30	1.47	1.37
1	A	482	VAL	CB-CG1	5.20	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	LYS	CE-NZ	5.13	1.61	1.49
1	A	628	PHE	CE2-CZ	5.12	1.47	1.37
1	A	332	PHE	CG-CD2	5.11	1.46	1.38
1	A	645	GLU	CD-OE2	5.11	1.31	1.25
1	A	106	GLN	CD-OE1	5.10	1.35	1.24
1	A	948	PHE	CE1-CZ	5.04	1.47	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	TYR	C-N-CD	-12.55	93.00	120.60
1	A	35	TYR	C-N-CA	8.37	157.15	122.00
1	A	418	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	418	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	722	GLU	O-C-N	-6.73	111.93	122.70
1	A	722	GLU	CA-C-O	6.68	134.12	120.10
1	A	193	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	937	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	518	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	674	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	866	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	535	LEU	CA-CB-CG	5.08	127.00	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	TYR	Peptide
1	A	388	PHE	Mainchain
1	A	469	GLN	Peptide
1	A	89	GLN	Sidechain

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	7718	0	7878	346	16

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7718	0	7878	346	16

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 22.

All (346) 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:110:LYS:NZ	1:A:110:LYS:CE	1.70	1.51
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.18	1.16
1:A:1022:VAL:HB	1:A:1023:PRO:CD	1.82	1.09
1:A:8:ARG:HB2	1:A:9:PRO:HD3	1.29	1.08
1:A:861:GLY:HA3	1:A:862:MET:HB3	1.35	1.07
1:A:680:PHE:HA	1:A:862:MET:HG3	1.27	1.06
1:A:454:VAL:HG23	1:A:455:PRO:HD3	1.39	1.04
1:A:851:LEU:HB2	1:A:852:PRO:HD2	1.40	1.02
1:A:545:TYR:HB2	1:A:1022:VAL:HG11	1.39	1.02
1:A:450:SER:HA	1:A:453:PHE:HB2	1.39	1.00
1:A:8:ARG:HB2	1:A:9:PRO:CD	1.91	1.00
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.46	0.95
1:A:475:VAL:HA	1:A:478:MET:HG3	1.46	0.95
1:A:445:ILE:HG13	1:A:446:ALA:H	1.30	0.94
1:A:453:PHE:O	1:A:455:PRO:HD2	1.67	0.94
1:A:861:GLY:HA3	1:A:862:MET:CB	2.01	0.90
1:A:473:THR:HA	1:A:476:SER:HB2	1.53	0.90
1:A:8:ARG:CB	1:A:9:PRO:HD3	2.01	0.90
1:A:454:VAL:HG23	1:A:455:PRO:CD	2.03	0.89
1:A:448:VAL:HG11	1:A:887:CYS:HB2	1.57	0.87
1:A:864:TYR:HB3	1:A:867:ARG:HG3	1.58	0.86
1:A:470:PHE:CG	1:A:473:THR:HB	2.12	0.85
1:A:352:PHE:HB3	1:A:369:THR:HG21	1.58	0.84
1:A:448:VAL:CG1	1:A:887:CYS:HB2	2.06	0.84
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.59	0.84
1:A:877:TYR:OH	1:A:932:LEU:HD11	1.78	0.83
1:A:302:THR:H	1:A:303:ALA:HB3	1.43	0.83
1:A:482:VAL:O	1:A:486:LEU:HB2	1.81	0.81
1:A:446:ALA:O	1:A:450:SER:HB3	1.79	0.81
1:A:864:TYR:HD2	1:A:866:GLU:H	1.32	0.78
1:A:446:ALA:HB3	1:A:478:MET:SD	2.24	0.78
1:A:722:GLU:O	1:A:723:ASP:HB2	1.82	0.77
1:A:968:VAL:HG11	1:A:1025:PHE:HE2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PHE:HA	1:A:862:MET:CG	2.13	0.77
1:A:892:TYR:HB3	1:A:897:ILE:HG13	1.67	0.77
1:A:497:LEU:O	1:A:498:LYS:HB3	1.86	0.76
1:A:410:ILE:HG21	1:A:978:THR:OG1	1.85	0.76
1:A:166:ILE:O	1:A:169:THR:HG22	1.87	0.74
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.68	0.74
1:A:900:SER:HB2	1:A:1027:VAL:HB	1.68	0.74
1:A:472:ILE:O	1:A:474:ILE:N	2.21	0.73
1:A:465:ALA:HB1	1:A:468:ARG:HB3	1.69	0.73
1:A:137:LEU:HD11	1:A:293:LEU:HD23	1.71	0.73
1:A:450:SER:CA	1:A:453:PHE:HB2	2.16	0.72
1:A:1012:VAL:HA	1:A:1015:THR:HG22	1.72	0.71
1:A:470:PHE:CD2	1:A:473:THR:HB	2.25	0.71
1:A:574:THR:HA	1:A:665:ALA:HA	1.73	0.71
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.71	0.70
1:A:982:PHE:O	1:A:984:LEU:N	2.22	0.70
1:A:873:ALA:H	1:A:874:PRO:CD	2.05	0.70
1:A:465:ALA:O	1:A:469:GLN:N	2.24	0.69
1:A:831:ALA:HB1	1:A:836:SER:HA	1.74	0.69
1:A:332:PHE:C	1:A:332:PHE:CD2	2.66	0.69
1:A:861:GLY:CA	1:A:862:MET:HB3	2.17	0.69
1:A:445:ILE:HG13	1:A:446:ALA:N	2.06	0.69
1:A:302:THR:N	1:A:303:ALA:HB3	2.06	0.69
1:A:357:LEU:O	1:A:358:PHE:HB2	1.92	0.69
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.75	0.69
1:A:472:ILE:O	1:A:475:VAL:N	2.26	0.68
1:A:426:PRO:HB2	1:A:427:PRO:HD3	1.77	0.67
1:A:892:TYR:CB	1:A:897:ILE:HG13	2.26	0.66
1:A:11:PHE:O	1:A:13:TRP:N	2.28	0.66
1:A:466:ILE:HA	1:A:469:GLN:HG2	1.78	0.65
1:A:911:GLY:HA2	1:A:914:LEU:H	1.61	0.65
1:A:911:GLY:HA3	1:A:914:LEU:HB2	1.78	0.65
1:A:926:TYR:HB3	1:A:1003:VAL:HG23	1.79	0.65
1:A:156:ASP:HA	1:A:181:GLN:HA	1.79	0.65
1:A:355:MET:HB3	1:A:365:THR:HG22	1.78	0.64
1:A:675:GLY:HA3	1:A:867:ARG:HH22	1.63	0.64
1:A:169:THR:HG23	1:A:170:SER:H	1.63	0.63
1:A:36:PRO:CD	1:A:391:ASN:HB3	2.27	0.63
1:A:188:MET:N	1:A:775:SER:HA	2.13	0.63
1:A:390:ILE:HG22	1:A:390:ILE:O	1.97	0.63
1:A:552:MET:HG3	1:A:913:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:PHE:H	1:A:1027:VAL:HG22	1.63	0.63
1:A:864:TYR:HB2	1:A:865:GLN:C	2.19	0.63
1:A:475:VAL:HA	1:A:478:MET:CG	2.26	0.62
1:A:375:VAL:HG21	1:A:405:LEU:HB2	1.81	0.62
1:A:353:LEU:C	1:A:355:MET:H	2.02	0.62
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.29	0.62
1:A:36:PRO:HD3	1:A:391:ASN:HB3	1.81	0.61
1:A:463:THR:HG23	1:A:867:ARG:HD2	1.82	0.61
1:A:730:ASP:HB3	1:A:806:SER:HB3	1.82	0.61
1:A:119:PRO:O	1:A:122:VAL:HG12	2.00	0.61
1:A:873:ALA:O	1:A:877:TYR:HD1	1.84	0.61
1:A:864:TYR:HB2	1:A:866:GLU:N	2.15	0.61
1:A:450:SER:HA	1:A:453:PHE:CB	2.24	0.61
1:A:456:MET:HB2	1:A:471:SER:OG	2.01	0.61
1:A:634:TRP:HA	1:A:637:ARG:HE	1.66	0.60
1:A:462:SER:C	1:A:464:GLY:H	2.05	0.60
1:A:446:ALA:O	1:A:450:SER:CB	2.48	0.60
1:A:360:GLN:O	1:A:361:ASN:HB2	2.01	0.60
1:A:392:THR:C	1:A:394:THR:H	2.05	0.60
1:A:178:PHE:HB2	1:A:288:GLY:H	1.67	0.60
1:A:462:SER:HB3	1:A:867:ARG:HD3	1.83	0.60
1:A:188:MET:H	1:A:775:SER:HA	1.67	0.60
1:A:438:ILE:O	1:A:442:LEU:HB2	2.02	0.59
1:A:910:ILE:O	1:A:913:LEU:HD12	2.03	0.59
1:A:1022:VAL:CB	1:A:1023:PRO:HD3	2.11	0.59
1:A:144:ASN:HA	1:A:320:GLY:O	2.03	0.59
1:A:347:ALA:O	1:A:351:VAL:HG23	2.03	0.58
1:A:450:SER:OG	1:A:454:VAL:HG22	2.03	0.58
1:A:864:TYR:HB3	1:A:867:ARG:CG	2.31	0.58
1:A:18:ILE:C	1:A:20:MET:H	2.06	0.57
1:A:598:TYR:HB3	1:A:606:VAL:HG11	1.87	0.57
1:A:426:PRO:HB2	1:A:427:PRO:CD	2.34	0.57
1:A:439:GLN:HG3	1:A:440:GLY:H	1.69	0.57
1:A:640:GLU:HA	1:A:643:LYS:HD2	1.87	0.57
1:A:949:ALA:O	1:A:951:ASP:N	2.39	0.56
1:A:332:PHE:HD2	1:A:332:PHE:C	2.09	0.56
1:A:453:PHE:O	1:A:455:PRO:CD	2.50	0.56
1:A:169:THR:HG23	1:A:170:SER:N	2.21	0.56
1:A:182:TYR:CD1	1:A:271:GLY:HA2	2.41	0.56
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.88	0.55
1:A:448:VAL:HG13	1:A:887:CYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HA	1:A:396:PHE:HB3	1.88	0.55
1:A:327:TYR:CD2	1:A:571:VAL:HG11	2.41	0.55
1:A:189:ASN:O	1:A:193:LEU:HB2	2.06	0.55
1:A:930:GLY:HA2	1:A:933:THR:HG22	1.87	0.55
1:A:959:GLY:HA3	1:A:963:ALA:HB2	1.89	0.55
1:A:925:VAL:O	1:A:925:VAL:HG12	2.07	0.55
1:A:472:ILE:HG12	1:A:473:THR:H	1.72	0.55
1:A:897:ILE:N	1:A:898:PRO:CD	2.70	0.55
1:A:831:ALA:O	1:A:832:ALA:CB	2.55	0.55
1:A:915:ALA:HB1	1:A:1005:THR:HG22	1.89	0.54
1:A:616:GLY:HA3	1:A:624:THR:HB	1.88	0.54
1:A:937:LEU:HD21	1:A:1011:MET:CE	2.37	0.54
1:A:713:LEU:O	1:A:832:ALA:HB2	2.07	0.54
1:A:937:LEU:HD21	1:A:1011:MET:HE1	1.89	0.54
1:A:389:SER:O	1:A:390:ILE:HB	2.08	0.54
1:A:531:VAL:O	1:A:534:ILE:HG22	2.07	0.53
1:A:38:ILE:HG21	1:A:466:ILE:HD11	1.90	0.53
1:A:470:PHE:CD1	1:A:472:ILE:HG23	2.43	0.53
1:A:18:ILE:HG22	1:A:19:ILE:H	1.72	0.53
1:A:299:ALA:O	1:A:303:ALA:HB3	2.08	0.53
1:A:1033:PHE:C	1:A:1035:ARG:H	2.13	0.53
1:A:473:THR:O	1:A:477:ALA:N	2.42	0.53
1:A:587:THR:HG23	1:A:613:ASN:HD21	1.73	0.53
1:A:532:GLY:O	1:A:536:ARG:HB2	2.09	0.53
1:A:843:LEU:O	1:A:847:LEU:HG	2.09	0.53
1:A:964:THR:O	1:A:968:VAL:HG22	2.09	0.52
1:A:873:ALA:O	1:A:877:TYR:CD1	2.62	0.52
1:A:123:GLN:C	1:A:125:GLN:H	2.11	0.52
1:A:478:MET:HE3	1:A:479:ALA:HB2	1.90	0.52
1:A:861:GLY:CA	1:A:862:MET:CB	2.79	0.52
1:A:367:ILE:HG13	1:A:492:LEU:HD12	1.89	0.52
1:A:863:SER:O	1:A:865:GLN:HA	2.10	0.52
1:A:451:ALA:HB1	1:A:880:SER:O	2.10	0.52
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.92	0.51
1:A:859:TRP:HB3	1:A:862:MET:CE	2.40	0.51
1:A:864:TYR:HB2	1:A:865:GLN:CA	2.40	0.51
1:A:548:ILE:HG23	1:A:910:ILE:HD11	1.91	0.51
1:A:851:LEU:HB2	1:A:852:PRO:CD	2.26	0.51
1:A:445:ILE:HB	1:A:449:LEU:HD21	1.92	0.51
1:A:764:ASP:HB3	1:A:769:LYS:HD3	1.91	0.51
1:A:126:GLY:O	1:A:127:VAL:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:SER:C	1:A:464:GLY:N	2.63	0.51
1:A:199:THR:HG23	1:A:202:ASP:H	1.75	0.51
1:A:680:PHE:CA	1:A:862:MET:HG3	2.20	0.51
1:A:426:PRO:CB	1:A:427:PRO:HD3	2.40	0.51
1:A:187:TRP:HE1	1:A:269:GLU:HG2	1.75	0.51
1:A:353:LEU:O	1:A:355:MET:N	2.44	0.51
1:A:342:LYS:O	1:A:346:GLU:HG3	2.11	0.51
1:A:472:ILE:CG1	1:A:473:THR:N	2.74	0.50
1:A:968:VAL:HA	1:A:971:ARG:NH2	2.26	0.50
1:A:637:ARG:HG2	1:A:637:ARG:O	2.11	0.50
1:A:453:PHE:N	1:A:453:PHE:CD2	2.79	0.50
1:A:911:GLY:N	1:A:912:ALA:HB3	2.26	0.50
1:A:864:TYR:CD2	1:A:866:GLU:N	2.76	0.50
1:A:438:ILE:HA	1:A:441:ALA:HB3	1.94	0.50
1:A:877:TYR:O	1:A:881:LEU:HB2	2.10	0.50
1:A:488:LEU:O	1:A:490:PRO:HD2	2.11	0.50
1:A:317:PHE:HE2	1:A:323:ILE:HD11	1.76	0.50
1:A:240:LEU:HD22	1:A:245:GLU:HB3	1.94	0.50
1:A:678:THR:O	1:A:831:ALA:HB2	2.11	0.50
1:A:742:SER:O	1:A:746:ILE:HD12	2.11	0.50
1:A:680:PHE:CD1	1:A:859:TRP:HZ3	2.30	0.50
1:A:299:ALA:O	1:A:302:THR:N	2.44	0.50
1:A:664:PHE:O	1:A:665:ALA:HB3	2.11	0.50
1:A:872:GLN:HG3	1:A:872:GLN:O	2.12	0.50
1:A:172:VAL:HG11	1:A:175:VAL:HG22	1.94	0.49
1:A:959:GLY:HA3	1:A:963:ALA:CB	2.42	0.49
1:A:949:ALA:O	1:A:952:LEU:N	2.31	0.49
1:A:34:GLN:HG3	1:A:35:TYR:H	1.77	0.49
1:A:1026:PHE:HB3	1:A:1030:ARG:HD3	1.95	0.49
1:A:886:LEU:C	1:A:888:LEU:H	2.16	0.49
1:A:211:ASN:HD22	1:A:760:ASN:HD21	1.61	0.49
1:A:350:LEU:HD21	1:A:984:LEU:HB2	1.93	0.49
1:A:470:PHE:HD1	1:A:472:ILE:HG23	1.77	0.49
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.95	0.49
1:A:377:LEU:HA	1:A:380:PHE:CZ	2.48	0.49
1:A:541:TYR:HB3	1:A:1022:VAL:HG13	1.95	0.48
1:A:887:CYS:C	1:A:889:ALA:H	2.16	0.48
1:A:65:ILE:HD11	1:A:118:LEU:HD11	1.94	0.48
1:A:61:VAL:HG11	1:A:122:VAL:HG21	1.95	0.48
1:A:562:SER:HB2	1:A:922:THR:HG23	1.94	0.48
1:A:1018:ALA:O	1:A:1024:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:LEU:HD11	1:A:855:VAL:HG11	1.95	0.48
1:A:392:THR:O	1:A:393:LEU:HB3	2.13	0.48
1:A:448:VAL:HG11	1:A:886:LEU:O	2.14	0.48
1:A:61:VAL:HG12	1:A:118:LEU:HD22	1.95	0.48
1:A:820:ASN:N	1:A:820:ASN:HD22	2.11	0.48
1:A:722:GLU:HB3	1:A:724:THR:HG23	1.95	0.48
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.96	0.48
1:A:563:PHE:HB3	1:A:564:LEU:H	1.48	0.48
1:A:438:ILE:HG22	1:A:442:LEU:HB2	1.95	0.47
1:A:931:LEU:O	1:A:935:ILE:HG12	2.14	0.47
1:A:584:GLN:H	1:A:622:GLN:HE21	1.61	0.47
1:A:991:ILE:C	1:A:993:THR:H	2.17	0.47
1:A:183:ALA:HB3	1:A:185:ARG:HD3	1.95	0.47
1:A:641:GLU:O	1:A:650:ARG:NH2	2.48	0.47
1:A:939:ALA:O	1:A:943:ILE:HG22	2.13	0.47
1:A:390:ILE:CG2	1:A:390:ILE:O	2.62	0.47
1:A:907:LEU:HD21	1:A:1023:PRO:HD2	1.97	0.47
1:A:400:LEU:HD13	1:A:1003:VAL:HG22	1.96	0.47
1:A:92:LEU:HD22	1:A:107:VAL:HG22	1.97	0.47
1:A:1023:PRO:O	1:A:1024:VAL:C	2.53	0.47
1:A:968:VAL:HG11	1:A:1025:PHE:CE2	2.38	0.47
1:A:262:LEU:HA	1:A:265:VAL:HG12	1.97	0.47
1:A:987:MET:N	1:A:988:PRO:CD	2.78	0.46
1:A:859:TRP:HE3	1:A:862:MET:HE1	1.80	0.46
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.96	0.46
1:A:353:LEU:C	1:A:355:MET:N	2.68	0.46
1:A:392:THR:HG22	1:A:393:LEU:H	1.80	0.46
1:A:36:PRO:HD3	1:A:391:ASN:CB	2.44	0.46
1:A:131:LYS:HD2	1:A:295:THR:HB	1.97	0.46
1:A:675:GLY:HA3	1:A:867:ARG:NH2	2.31	0.46
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.98	0.46
1:A:859:TRP:HB3	1:A:862:MET:HE1	1.97	0.46
1:A:863:SER:C	1:A:864:TYR:CG	2.89	0.46
1:A:944:LEU:HD13	1:A:948:PHE:CD1	2.51	0.46
1:A:324:VAL:HG23	1:A:326:PRO:HD3	1.98	0.46
1:A:29:LYS:HB3	1:A:32:VAL:HG23	1.97	0.45
1:A:453:PHE:HD2	1:A:453:PHE:N	2.12	0.45
1:A:392:THR:C	1:A:394:THR:N	2.69	0.45
1:A:1026:PHE:CD1	1:A:1026:PHE:N	2.85	0.45
1:A:978:THR:C	1:A:980:LEU:H	2.20	0.45
1:A:976:LEU:O	1:A:980:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:THR:HG23	1:A:988:PRO:HB2	1.99	0.45
1:A:24:GLY:O	1:A:27:ILE:HG22	2.16	0.45
1:A:453:PHE:HB3	1:A:475:VAL:HG23	1.98	0.45
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.98	0.45
1:A:680:PHE:CD1	1:A:680:PHE:C	2.90	0.45
1:A:477:ALA:O	1:A:481:SER:N	2.36	0.45
1:A:575:MET:HB3	1:A:664:PHE:HB2	1.98	0.45
1:A:911:GLY:HA2	1:A:912:ALA:C	2.37	0.45
1:A:425:LEU:HA	1:A:426:PRO:HD3	1.74	0.45
1:A:571:VAL:HG22	1:A:630:SER:HA	1.99	0.45
1:A:435:MET:CE	1:A:490:PRO:HB3	2.47	0.45
1:A:862:MET:SD	1:A:863:SER:N	2.90	0.45
1:A:384:ALA:HB2	1:A:390:ILE:CD1	2.47	0.45
1:A:760:ASN:HD22	1:A:760:ASN:C	2.20	0.45
1:A:939:ALA:O	1:A:943:ILE:N	2.50	0.45
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.98	0.44
1:A:774:MET:O	1:A:775:SER:CB	2.64	0.44
1:A:990:VAL:HG23	1:A:991:ILE:HG13	1.99	0.44
1:A:668:LEU:HA	1:A:669:PRO:HD3	1.78	0.44
1:A:831:ALA:O	1:A:832:ALA:HB2	2.16	0.44
1:A:727:PHE:HZ	1:A:807:SER:HB3	1.82	0.44
1:A:302:THR:CA	1:A:303:ALA:HB3	2.47	0.44
1:A:459:PHE:HE1	1:A:468:ARG:HD2	1.82	0.44
1:A:409:ALA:O	1:A:413:VAL:HG23	2.17	0.44
1:A:61:VAL:O	1:A:65:ILE:HG12	2.17	0.44
1:A:739:LEU:HD12	1:A:741:VAL:HG22	1.99	0.44
1:A:873:ALA:N	1:A:874:PRO:CD	2.75	0.44
1:A:361:ASN:O	1:A:365:THR:HG23	2.18	0.44
1:A:942:ALA:O	1:A:945:ILE:HG13	2.17	0.44
1:A:968:VAL:HA	1:A:971:ARG:CZ	2.48	0.43
1:A:402:ILE:O	1:A:402:ILE:CG2	2.66	0.43
1:A:140:VAL:HG12	1:A:323:ILE:HG22	2.00	0.43
1:A:562:SER:N	1:A:923:ASN:O	2.51	0.43
1:A:302:THR:HB	1:A:303:ALA:CB	2.48	0.43
1:A:721:LEU:HD23	1:A:722:GLU:N	2.33	0.43
1:A:831:ALA:HA	1:A:840:ALA:CB	2.48	0.43
1:A:33:ALA:CB	1:A:299:ALA:HB3	2.49	0.43
1:A:27:ILE:C	1:A:29:LYS:H	2.21	0.43
1:A:446:ALA:HA	1:A:449:LEU:HG	2.00	0.43
1:A:655:PHE:HB3	1:A:663:VAL:CG2	2.48	0.43
1:A:448:VAL:HA	1:A:883:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:PHE:HD1	1:A:1026:PHE:N	2.16	0.43
1:A:569:GLN:HG3	1:A:668:LEU:HB3	2.00	0.43
1:A:836:SER:O	1:A:838:GLY:N	2.52	0.43
1:A:451:ALA:HB3	1:A:884:VAL:HG23	2.01	0.43
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.19	0.43
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.43
1:A:203:VAL:O	1:A:207:ILE:HG12	2.19	0.43
1:A:664:PHE:O	1:A:665:ALA:CB	2.67	0.42
1:A:646:ALA:HA	1:A:649:MET:HB2	2.00	0.42
1:A:888:LEU:O	1:A:897:ILE:HB	2.19	0.42
1:A:975:ILE:HG22	1:A:975:ILE:O	2.19	0.42
1:A:835:LYS:HD2	1:A:839:GLU:HB2	2.01	0.42
1:A:454:VAL:CG2	1:A:455:PRO:CD	2.89	0.42
1:A:926:TYR:HB3	1:A:1003:VAL:HA	2.01	0.42
1:A:927:PHE:O	1:A:931:LEU:HB2	2.19	0.42
1:A:357:LEU:O	1:A:358:PHE:CB	2.64	0.42
1:A:8:ARG:CB	1:A:9:PRO:CD	2.72	0.42
1:A:472:ILE:HA	1:A:475:VAL:HB	2.01	0.42
1:A:402:ILE:O	1:A:402:ILE:HG23	2.20	0.42
1:A:475:VAL:HG13	1:A:478:MET:HE3	2.01	0.42
1:A:384:ALA:HB2	1:A:390:ILE:HD11	2.02	0.42
1:A:57:VAL:HG23	1:A:82:SER:HB2	2.00	0.42
1:A:1024:VAL:O	1:A:1025:PHE:HB2	2.20	0.42
1:A:302:THR:HB	1:A:303:ALA:HB2	2.02	0.42
1:A:332:PHE:HD2	1:A:332:PHE:O	2.03	0.42
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.54	0.42
1:A:1019:ILE:HG23	1:A:1020:PHE:CD2	2.55	0.42
1:A:911:GLY:HA2	1:A:913:LEU:N	2.34	0.42
1:A:446:ALA:CB	1:A:478:MET:SD	3.02	0.41
1:A:1033:PHE:HB2	1:A:1034:SER:H	1.64	0.41
1:A:116:PRO:HA	1:A:123:GLN:NE2	2.35	0.41
1:A:462:SER:HB3	1:A:867:ARG:CD	2.49	0.41
1:A:454:VAL:N	1:A:471:SER:HB3	2.35	0.41
1:A:575:MET:HA	1:A:626:ILE:HG22	2.02	0.41
1:A:214:VAL:HG22	1:A:237:GLN:HB2	2.02	0.41
1:A:261:LEU:O	1:A:263:ARG:N	2.53	0.41
1:A:685:ILE:HG23	1:A:824:SER:HB2	2.01	0.41
1:A:1011:MET:O	1:A:1015:THR:N	2.53	0.41
1:A:314:GLU:N	1:A:315:PRO:CD	2.83	0.41
1:A:602:GLU:HG2	1:A:605:ASN:HB2	2.02	0.41
1:A:151:GLN:HE22	1:A:279:ALA:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:H	1:A:346:GLU:HG3	1.77	0.41
1:A:473:THR:C	1:A:475:VAL:H	2.24	0.41
1:A:36:PRO:HD2	1:A:391:ASN:HB3	2.00	0.41
1:A:149:MET:O	1:A:150:THR:CB	2.68	0.41
1:A:1027:VAL:HG23	1:A:1028:VAL:HG23	2.02	0.41
1:A:906:PRO:O	1:A:910:ILE:HG12	2.21	0.41
1:A:944:LEU:O	1:A:948:PHE:HD1	2.04	0.41
1:A:690:LEU:HB3	1:A:694:LYS:HD2	2.02	0.41
1:A:478:MET:SD	1:A:479:ALA:N	2.93	0.41
1:A:318:PRO:HB2	1:A:319:SER:H	1.71	0.41
1:A:971:ARG:O	1:A:974:PRO:HD2	2.20	0.41
1:A:8:ARG:HE	1:A:8:ARG:H	1.68	0.41
1:A:34:GLN:O	1:A:392:THR:HB	2.21	0.41
1:A:36:PRO:HD3	1:A:391:ASN:CG	2.41	0.40
1:A:380:PHE:HA	1:A:383:LEU:HG	2.02	0.40
1:A:946:VAL:HG13	1:A:1028:VAL:HG22	2.02	0.40
1:A:438:ILE:O	1:A:438:ILE:HG22	2.21	0.40
1:A:372:VAL:HG23	1:A:373:PRO:HD3	2.03	0.40
1:A:554:TYR:C	1:A:556:PHE:H	2.25	0.40
1:A:873:ALA:H	1:A:874:PRO:HD2	1.82	0.40
1:A:36:PRO:HG3	1:A:469:GLN:NE2	2.36	0.40
1:A:898:PRO:O	1:A:902:MET:HG2	2.21	0.40
1:A:904:VAL:HG22	1:A:1023:PRO:HB3	2.03	0.40
1:A:442:LEU:O	1:A:445:ILE:HG12	2.21	0.40
1:A:98:THR:HB	1:A:99:ASP:H	1.65	0.40
1:A:915:ALA:O	1:A:919:ARG:HB3	2.21	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:CG	1:A:962:GLU:OE1[16_544]	1.47	0.73
1:A:536:ARG:NE	1:A:962:GLU:OE2[16_544]	1.57	0.63
1:A:228:GLN:OE1	1:A:781:MET:SD[2_545]	1.63	0.57
1:A:536:ARG:CG	1:A:962:GLU:CD[16_544]	1.67	0.53
1:A:70:ASN:CB	1:A:167:SER:OG[3_655]	1.79	0.41
1:A:14:VAL:CG1	1:A:886:LEU:CD1[2_545]	1.89	0.31
1:A:10:ILE:CG2	1:A:893:GLU:OE1[2_545]	1.90	0.30
1:A:536:ARG:CD	1:A:962:GLU:CD[16_544]	1.92	0.28
1:A:536:ARG:CG	1:A:962:GLU:OE2[16_544]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASN:ND2	1:A:167:SER:CB[3_655]	1.93	0.27
1:A:51:GLY:O	1:A:216:ALA:O[3_655]	1.97	0.23
1:A:112:GLN:NE2	1:A:112:GLN:NE2[2_545]	2.00	0.20
1:A:69:MET:O	1:A:168:ARG:CG[3_655]	2.02	0.18
1:A:536:ARG:CD	1:A:962:GLU:OE2[16_544]	2.03	0.17
1:A:536:ARG:NE	1:A:962:GLU:CD[16_544]	2.16	0.04
1:A:226:LYS:NZ	1:A:283:GLY:CA[5_545]	2.18	0.02

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	1012/1053 (96%)	776 (77%)	156 (15%)	80 (8%)	1 16

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	12	ALA
1	A	19	ILE
1	A	36	PRO
1	A	262	LEU
1	A	354	VAL
1	A	358	PHE
1	A	390	ILE
1	A	426	PRO
1	A	427	PRO
1	A	454	VAL
1	A	464	GLY
1	A	470	PHE
1	A	472	ILE
1	A	473	THR
1	A	489	THR

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Mol	Chain	Res	Type
1	A	539	GLY
1	A	665	ALA
1	A	832	ALA
1	A	837	THR
1	A	873	ALA
1	A	921	LEU
1	A	950	LYS
1	A	982	PHE
1	A	1022	VAL
1	A	1023	PRO
1	A	9	PRO
1	A	32	VAL
1	A	127	VAL
1	A	150	THR
1	A	361	ASN
1	A	389	SER
1	A	563	PHE
1	A	674	LEU
1	A	775	SER
1	A	852	PRO
1	A	861	GLY
1	A	867	ARG
1	A	887	CYS
1	A	983	ILE
1	A	1024	VAL
1	A	1025	PHE
1	A	98	THR
1	A	318	PRO
1	A	385	ALA
1	A	419	VAL
1	A	455	PRO
1	A	538	THR
1	A	615	PHE
1	A	675	GLY
1	A	721	LEU
1	A	864	TYR
1	A	866	GLU
1	A	75	LEU
1	A	294	ALA
1	A	297	ALA
1	A	300	LEU
1	A	303	ALA

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Mol	Chain	Res	Type
1	A	360	GLN
1	A	461	GLY
1	A	566	ASP
1	A	579	PRO
1	A	638	PRO
1	A	677	ALA
1	A	874	PRO
1	A	898	PRO
1	A	8	ARG
1	A	146	ASP
1	A	226	LYS
1	A	428	LYS
1	A	671	ILE
1	A	151	GLN
1	A	759	VAL
1	A	968	VAL
1	A	445	ILE
1	A	783	PRO
1	A	272	GLY
1	A	959	GLY
1	A	911	GLY
1	A	31	PRO

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	826/858 (96%)	698 (84%)	128 (16%)	3 22

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	ILE
1	A	11	PHE
1	A	13	TRP

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Mol	Chain	Res	Type
1	A	25	LEU
1	A	45	ILE
1	A	49	TYR
1	A	72	ILE
1	A	84	SER
1	A	104	GLN
1	A	108	GLN
1	A	110	LYS
1	A	113	LEU
1	A	120	GLN
1	A	123	GLN
1	A	124	GLN
1	A	125	GLN
1	A	140	VAL
1	A	143	ILE
1	A	161	ASN
1	A	176	GLN
1	A	177	LEU
1	A	180	SER
1	A	205	THR
1	A	208	LYS
1	A	210	GLN
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	239	ARG
1	A	252	LYS
1	A	261	LEU
1	A	277	ILE
1	A	278	ILE
1	A	293	LEU
1	A	298	ASN
1	A	301	ASP
1	A	306	ILE
1	A	327	TYR
1	A	332	PHE
1	A	343	THR
1	A	346	GLU
1	A	350	LEU
1	A	355	MET
1	A	356	TYR
1	A	357	LEU

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Mol	Chain	Res	Type
1	A	362	PHE
1	A	366	LEU
1	A	386	PHE
1	A	390	ILE
1	A	398	MET
1	A	402	ILE
1	A	415	ASN
1	A	417	GLU
1	A	418	ARG
1	A	420	MET
1	A	423	GLU
1	A	425	LEU
1	A	431	THR
1	A	442	LEU
1	A	449	LEU
1	A	453	PHE
1	A	456	MET
1	A	458	PHE
1	A	471	SER
1	A	472	ILE
1	A	473	THR
1	A	478	MET
1	A	492	LEU
1	A	498	LYS
1	A	516	PHE
1	A	519	MET
1	A	520	PHE
1	A	535	LEU
1	A	563	PHE
1	A	566	ASP
1	A	567	GLU
1	A	568	ASP
1	A	569	GLN
1	A	601	LYS
1	A	632	LYS
1	A	637	ARG
1	A	643	LYS
1	A	650	ARG
1	A	659	LYS
1	A	662	MET
1	A	663	VAL
1	A	674	LEU

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Mol	Chain	Res	Type
1	A	680	PHE
1	A	687	GLN
1	A	696	THR
1	A	697	GLN
1	A	702	LEU
1	A	714	THR
1	A	721	LEU
1	A	723	ASP
1	A	760	ASN
1	A	797	GLN
1	A	804	PHE
1	A	815	ARG
1	A	843	LEU
1	A	846	GLN
1	A	853	THR
1	A	855	VAL
1	A	860	THR
1	A	864	TYR
1	A	867	ARG
1	A	902	MET
1	A	903	LEU
1	A	907	LEU
1	A	913	LEU
1	A	919	ARG
1	A	923	ASN
1	A	937	LEU
1	A	940	LYS
1	A	943	ILE
1	A	944	LEU
1	A	948	PHE
1	A	953	MET
1	A	970	MET
1	A	971	ARG
1	A	972	LEU
1	A	1011	MET
1	A	1015	THR
1	A	1021	PHE
1	A	1022	VAL
1	A	1026	PHE
1	A	1033	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	125	GLN
1	A	151	GLN
1	A	176	GLN
1	A	194	ASN
1	A	210	GLN
1	A	218	GLN
1	A	231	ASN
1	A	284	GLN
1	A	361	ASN
1	A	415	ASN
1	A	469	GLN
1	A	517	ASN
1	A	604	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	687	GLN
1	A	760	ASN
1	A	820	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	1016/1053 (96%)	0.18	39 (3%) 44 36	16, 84, 152, 191	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	5.0
1	A	829	GLY	4.4
1	A	960	LEU	4.4
1	A	295	THR	4.2
1	A	833	PRO	3.6
1	A	425	LEU	3.6
1	A	543	VAL	3.4
1	A	1021	PHE	3.4
1	A	31	PRO	3.2
1	A	525	HIS	3.0
1	A	400	LEU	2.8
1	A	496	MET	2.7
1	A	676	THR	2.7
1	A	677	ALA	2.7
1	A	944	LEU	2.6
1	A	408	ASP	2.5
1	A	405	LEU	2.5
1	A	712	MET	2.5
1	A	678	THR	2.4
1	A	827	ILE	2.4
1	A	517	ASN	2.4
1	A	722	GLU	2.4
1	A	401	ALA	2.3
1	A	460	GLY	2.3
1	A	834	GLY	2.2
1	A	830	GLN	2.2
1	A	363	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	804	PHE	2.1
1	A	406	VAL	2.1
1	A	461	GLY	2.1
1	A	426	PRO	2.1
1	A	492	LEU	2.0
1	A	362	PHE	2.0
1	A	711	ASP	2.0
1	A	872	GLN	2.0
1	A	334	LYS	2.0
1	A	306	ILE	2.0
1	A	437	GLN	2.0
1	A	992	SER	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.