W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2018 – 07:42 PM EST

PDB ID	:	1D1A
Title	:	DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT) COMPLEXED WITH O,P-DINITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE.
Authors	:	Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on	:	1999-09-15
Resolution	:	2.00 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 (i)) were used in the production of this report:

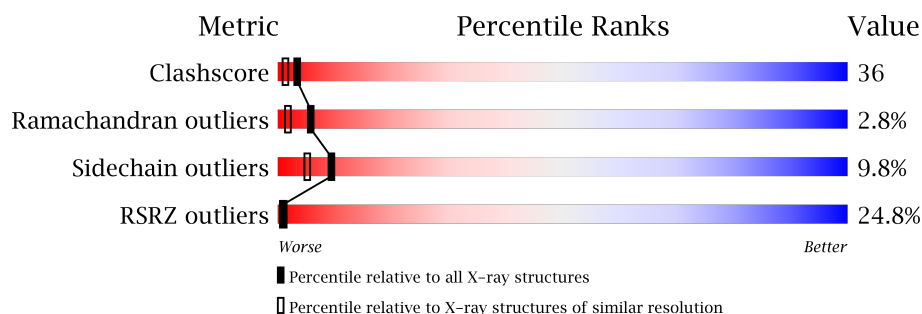|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 2.00 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	Percentile Ranks	Value
Clashscore		36
Ramachandran outliers		2.8%
Sidechain outliers		9.8%
RSRZ outliers		24.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	761	24% / 45% / 40% / 11% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6235 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	745	Total 5772	C 3660	N 994	O 1102	S 16	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	ENGINEERED	UNP P08799
A	761	ASN	ARG	ENGINEERED	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

- Molecule 3 is O,P-DINITROPHENYL AMINOETHYLDIPHOSPHATE-BERYLLIUM TRIFLUORIDE (three-letter code: DAE) (formula: $C_8H_{10}BeF_3N_3O_{11}P_2$).

DAE
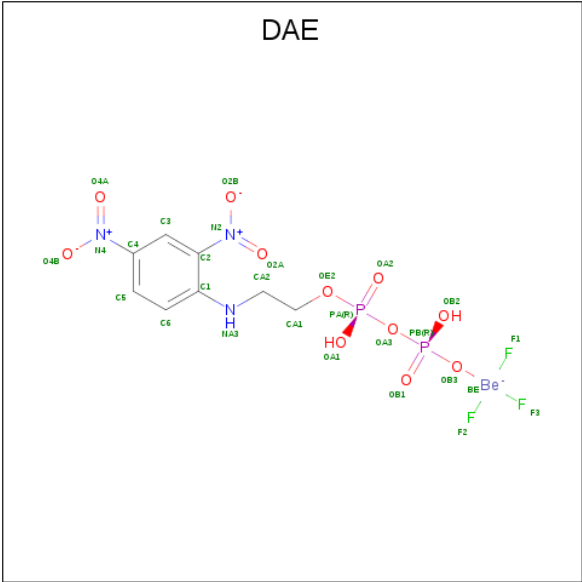
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Be	C	F	N	O	P	0	0
			28	1	8	3	3	11	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	434	Total	O	0	0
			434	434		

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 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: MYOSIN
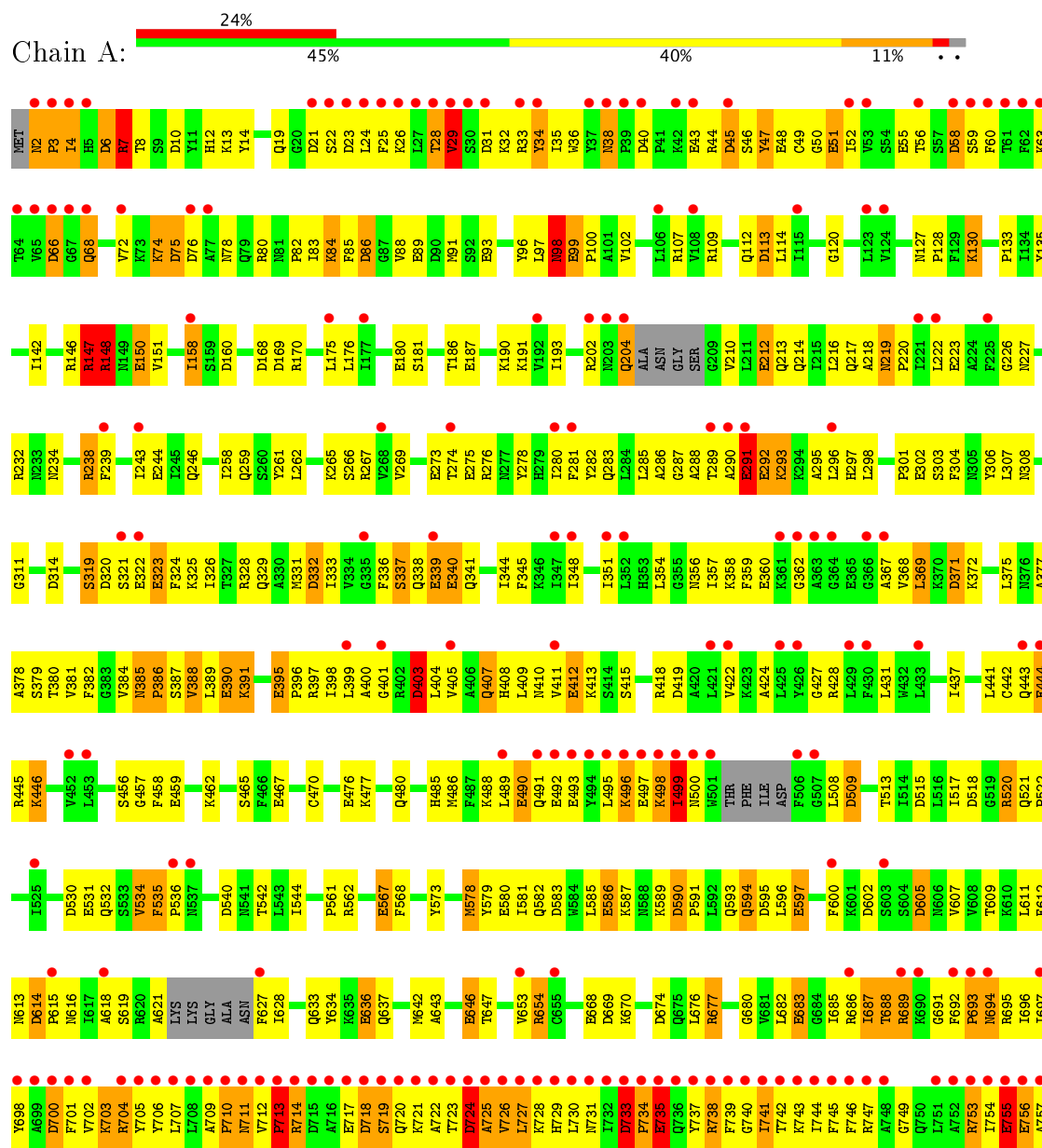
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.73Å　　180.00Å　　54.02Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	25.00　–　2.00 29.96　–　2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-2.00) 96.8 (29.96-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.00Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.226　,　(Not available) 0.249　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 166.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.93	38/5882 (0.6%)	1.38	74/7967 (0.9%)

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	2	0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	GLU	CD-OE2	7.05	1.33	1.25
1	A	302	GLU	CD-OE2	6.74	1.33	1.25
1	A	89	GLU	CD-OE2	6.57	1.32	1.25
1	A	275	GLU	CD-OE2	6.57	1.32	1.25
1	A	490	GLU	CD-OE2	6.41	1.32	1.25
1	A	756	GLU	CD-OE2	6.27	1.32	1.25
1	A	717	GLU	CD-OE2	6.27	1.32	1.25
1	A	93	GLU	CD-OE2	6.26	1.32	1.25
1	A	48	GLU	CD-OE2	6.21	1.32	1.25
1	A	291	GLU	CD-OE2	6.18	1.32	1.25
1	A	444	GLU	CD-OE2	6.08	1.32	1.25
1	A	99	GLU	CD-OE2	6.04	1.32	1.25
1	A	412	GLU	CD-OE2	6.03	1.32	1.25
1	A	646	GLU	CD-OE2	6.00	1.32	1.25
1	A	150	GLU	CD-OE2	5.98	1.32	1.25
1	A	476	GLU	CD-OE2	5.98	1.32	1.25
1	A	567	GLU	CD-OE2	5.81	1.32	1.25
1	A	51	GLU	CD-OE2	5.80	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	GLU	CD-OE2	5.78	1.32	1.25
1	A	55	GLU	CD-OE2	5.72	1.31	1.25
1	A	531	GLU	CD-OE2	5.71	1.31	1.25
1	A	668	GLU	CD-OE2	5.71	1.31	1.25
1	A	586	GLU	CD-OE2	5.68	1.31	1.25
1	A	187	GLU	CD-OE2	5.66	1.31	1.25
1	A	292	GLU	CD-OE2	5.65	1.31	1.25
1	A	323	GLU	CD-OE2	5.63	1.31	1.25
1	A	459	GLU	CD-OE2	5.62	1.31	1.25
1	A	340	GLU	CD-OE2	5.62	1.31	1.25
1	A	597	GLU	CD-OE2	5.58	1.31	1.25
1	A	212	GLU	CD-OE2	5.52	1.31	1.25
1	A	180	GLU	CD-OE2	5.48	1.31	1.25
1	A	390	GLU	CD-OE2	5.47	1.31	1.25
1	A	395	GLU	CD-OE2	5.47	1.31	1.25
1	A	244	GLU	CD-OE2	5.38	1.31	1.25
1	A	636	GLU	CD-OE2	5.35	1.31	1.25
1	A	360	GLU	CD-OE2	5.30	1.31	1.25
1	A	467	GLU	CD-OE2	5.24	1.31	1.25
1	A	735	GLU	CD-OE2	5.18	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	147	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	689	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	148	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	21	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	605	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	602	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	A	520	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	21	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	A	320	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	168	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	419	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	A	713	PRO	N-CA-CB	7.40	112.18	103.30
1	A	320	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	6	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	160	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	232	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	45	ASP	CB-CG-OD2	-7.03	111.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	674	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	168	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	530	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	704	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	219	ASN	CB-CA-C	6.55	123.50	110.40
1	A	66	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	509	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	371	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	6	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	160	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	700	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	605	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	520	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	602	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	718	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	385	ASN	C-N-CD	-6.15	107.06	120.60
1	A	238	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	403	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	674	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	518	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	590	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	76	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	45	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	34	TYR	N-CA-C	5.78	126.61	111.00
1	A	614	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	58	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	267	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	669	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	34	TYR	CB-CG-CD2	5.64	124.39	121.00
1	A	535	PHE	CA-CB-CG	-5.62	100.41	113.90
1	A	614	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	314	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	113	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	403	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	47	TYR	CB-CA-C	-5.51	99.38	110.40
1	A	700	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	583	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	515	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	530	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	595	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	562	ARG	NE-CZ-NH2	-5.35	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ASN	N-CA-CB	5.33	120.19	110.60
1	A	733	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	734	PRO	N-CA-CB	5.23	109.57	103.30
1	A	419	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	58	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	75	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	7	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	499	ILE	CB-CA-C	5.11	121.82	111.60
1	A	86	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	724	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	590	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	677	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	332	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	518	ASP	CB-CG-OD1	5.04	122.84	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	219	ASN	CA
1	A	499	ILE	CA

There are no planarity outliers.

5.2　Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5772	0	5502	403	0
2	A	1	0	0	0	0
3	A	28	0	8	3	0
4	A	434	0	0	19	0
All	All	6235	0	5510	404	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 36.

All (404) 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:398:ILE:HD13	1:A:407:GLN:HG3	1.39	1.04
1:A:98:ASN:HB2	1:A:100:PRO:HD2	1.41	1.02
1:A:443:GLN:CG	1:A:445:ARG:O	2.07	1.00
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.46	0.97
1:A:709:ALA:HB1	1:A:729:HIS:ND1	1.81	0.96
1:A:4:ILE:HD11	1:A:142:ILE:CG2	1.96	0.93
1:A:34:TYR:HB3	1:A:51:GLU:HA	1.51	0.92
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.05	0.91
1:A:711:ASN:HB2	1:A:729:HIS:CE1	2.08	0.89
1:A:619:SER:HB3	1:A:627:PHE:HE2	1.34	0.88
1:A:45:ASP:HB2	1:A:670:LYS:HG2	1.56	0.87
1:A:737:TYR:HB3	1:A:746:PHE:CE1	2.11	0.84
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.11	0.84
1:A:698:TYR:CD1	1:A:720:GLN:HG2	2.13	0.83
1:A:147:ARG:HG2	1:A:150:GLU:OE1	1.79	0.82
1:A:58:ASP:O	1:A:74:LYS:HB3	1.78	0.82
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.80	0.81
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.45	0.81
1:A:443:GLN:HG2	1:A:445:ARG:O	1.79	0.80
1:A:34:TYR:CB	1:A:51:GLU:HA	2.12	0.80
1:A:723:THR:HG22	1:A:739:PHE:HZ	1.44	0.80
1:A:372:LYS:HE3	1:A:390:GLU:OE1	1.82	0.80
1:A:337:SER:O	1:A:341:GLN:HG3	1.82	0.79
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.62	0.79
1:A:80:ARG:HH12	1:A:83:ILE:HG12	1.48	0.79
1:A:480:GLN:HG3	1:A:508:LEU:HD12	1.66	0.78
1:A:336:PHE:O	1:A:341:GLN:NE2	2.15	0.78
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.66	0.78
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.20	0.77
1:A:480:GLN:HG3	1:A:508:LEU:CD1	2.14	0.77
1:A:400:ALA:HB3	1:A:403:ASP:HB2	1.67	0.76
1:A:297:HIS:C	1:A:298:LEU:HD23	2.05	0.76
1:A:4:ILE:HD11	1:A:142:ILE:HG21	1.66	0.75
1:A:43:GLU:HB2	1:A:670:LYS:HZ2	1.50	0.75
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.66	0.75
1:A:35:ILE:HG12	1:A:36:TRP:N	2.02	0.75
1:A:702:VAL:HG23	1:A:712:VAL:CG1	2.17	0.75
1:A:735:GLU:HB3	1:A:747:ARG:NH2	2.02	0.74
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.02	0.74
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.17	0.74
1:A:158:ILE:HD12	1:A:175:LEU:HD23	1.68	0.74
1:A:733:ASP:O	1:A:737:TYR:CE2	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASP:HB3	1:A:581:ILE:HD13	1.69	0.74
1:A:396:PRO:O	1:A:398:ILE:HD12	1.88	0.73
1:A:107:ARG:HG3	4:A:1192:HOH:O	1.89	0.72
1:A:395:GLU:HA	1:A:407:GLN:O	1.89	0.72
1:A:210:VAL:O	1:A:214:GLN:HG3	1.89	0.72
1:A:377:ALA:O	1:A:380:THR:HG22	1.89	0.72
1:A:7:ARG:HD3	1:A:12:HIS:CE1	2.25	0.71
1:A:709:ALA:HB2	1:A:726:VAL:HG13	1.71	0.70
1:A:443:GLN:HG3	1:A:445:ARG:O	1.92	0.70
1:A:35:ILE:HG12	1:A:36:TRP:H	1.55	0.70
1:A:582:GLN:N	1:A:582:GLN:OE1	2.20	0.70
1:A:98:ASN:CB	1:A:100:PRO:HD2	2.21	0.70
1:A:146:ARG:HD3	1:A:151:VAL:HG13	1.72	0.70
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.92	0.69
1:A:491:GLN:O	1:A:495:LEU:HD13	1.91	0.69
1:A:687:ILE:HG22	1:A:688:THR:N	2.07	0.69
1:A:735:GLU:CB	1:A:747:ARG:HH21	2.05	0.69
1:A:380:THR:HG23	1:A:381:VAL:N	2.08	0.69
1:A:80:ARG:HH12	1:A:83:ILE:CG1	2.06	0.69
1:A:740:GLY:O	1:A:742:THR:N	2.25	0.68
1:A:38:ASN:OD1	1:A:44:ARG:HA	1.92	0.68
1:A:698:TYR:HH	1:A:739:PHE:HD2	1.41	0.68
1:A:753:ARG:HH21	1:A:757:ALA:HB2	1.58	0.68
1:A:80:ARG:HH12	1:A:83:ILE:CD1	2.06	0.67
1:A:702:VAL:HG23	1:A:712:VAL:HG11	1.75	0.67
1:A:293:LYS:O	1:A:296:LEU:N	2.26	0.67
1:A:325:LYS:O	1:A:329:GLN:HG3	1.94	0.67
1:A:738:ARG:O	1:A:744:ILE:HD12	1.95	0.67
1:A:544:ILE:HB	1:A:581:ILE:HG12	1.77	0.66
1:A:410:ASN:OD1	1:A:413:LYS:HB2	1.96	0.66
1:A:443:GLN:HG3	1:A:445:ARG:C	2.16	0.66
1:A:43:GLU:HB2	1:A:670:LYS:NZ	2.10	0.66
1:A:642:MET:O	1:A:646:GLU:HG2	1.96	0.66
1:A:695:ARG:HA	1:A:745:PHE:HA	1.77	0.66
1:A:686:ARG:O	1:A:689:ARG:HB3	1.95	0.66
1:A:694:ASN:N	1:A:694:ASN:ND2	2.44	0.66
1:A:385:ASN:O	1:A:388:VAL:HG23	1.95	0.66
1:A:34:TYR:CD1	1:A:49:CYS:SG	2.89	0.65
1:A:399:LEU:HG	1:A:401:GLY:H	1.61	0.65
1:A:273:GLU:O	1:A:274:THR:OG1	2.09	0.65
1:A:711:ASN:HB2	1:A:729:HIS:HE1	1.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ALA:CB	1:A:628:ILE:HG23	2.27	0.65
1:A:283:GLN:HB3	1:A:324:PHE:HB2	1.79	0.65
1:A:586:GLU:HB2	4:A:1399:HOH:O	1.97	0.65
1:A:12:HIS:ND1	4:A:1198:HOH:O	2.28	0.65
1:A:753:ARG:NE	1:A:753:ARG:O	2.30	0.65
1:A:246:GLN:OE1	1:A:443:GLN:HB3	1.97	0.64
1:A:580:GLU:HG3	1:A:580:GLU:O	1.96	0.64
1:A:158:ILE:CD1	1:A:175:LEU:HD23	2.26	0.64
1:A:298:LEU:HD23	1:A:298:LEU:N	2.12	0.64
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.80	0.64
1:A:753:ARG:HG3	1:A:753:ARG:HH11	1.63	0.64
1:A:43:GLU:HA	1:A:670:LYS:HZ1	1.64	0.63
1:A:293:LYS:O	1:A:297:HIS:N	2.31	0.63
1:A:753:ARG:HA	1:A:756:GLU:OE2	1.99	0.63
1:A:621:ALA:HB3	1:A:628:ILE:H	1.64	0.63
1:A:753:ARG:O	1:A:756:GLU:HB2	1.98	0.63
1:A:697:ILE:HG22	1:A:700:ASP:H	1.64	0.63
1:A:35:ILE:HG22	1:A:50:GLY:O	1.99	0.62
1:A:498:LYS:CB	1:A:741:ILE:HG13	2.29	0.62
1:A:338:GLN:HB3	1:A:339:GLU:OE1	2.00	0.62
1:A:698:TYR:HE2	1:A:739:PHE:CE2	2.17	0.62
1:A:698:TYR:CG	1:A:720:GLN:HG2	2.35	0.62
1:A:382:PHE:HB2	1:A:384:VAL:HG22	1.82	0.62
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.30	0.62
1:A:686:ARG:HA	1:A:689:ARG:HB2	1.82	0.62
1:A:490:GLU:HA	1:A:490:GLU:OE1	1.98	0.61
1:A:534:VAL:O	1:A:536:PRO:HD3	2.00	0.61
1:A:380:THR:HG23	1:A:381:VAL:H	1.66	0.61
1:A:698:TYR:O	1:A:702:VAL:HG12	1.99	0.61
1:A:296:LEU:CB	1:A:298:LEU:HG	2.27	0.61
1:A:7:ARG:NH1	1:A:12:HIS:HE1	1.99	0.61
1:A:2:ASN:ND2	1:A:4:ILE:H	1.99	0.60
1:A:495:LEU:HD12	1:A:495:LEU:N	2.17	0.60
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.36	0.60
1:A:443:GLN:CD	1:A:445:ARG:O	2.40	0.60
1:A:33:ARG:O	1:A:52:ILE:HB	2.01	0.60
1:A:34:TYR:HD1	1:A:49:CYS:SG	2.25	0.60
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.31	0.60
1:A:80:ARG:NH1	1:A:83:ILE:HG12	2.16	0.60
1:A:387:SER:O	1:A:391:LYS:HB2	2.01	0.60
1:A:130:LYS:HA	3:A:999:DAE:O4A	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:CG2	1:A:381:VAL:H	2.15	0.59
1:A:24:LEU:HB3	1:A:26:LYS:CB	2.33	0.59
1:A:713:PRO:O	1:A:714:ARG:O	2.21	0.59
1:A:219:ASN:N	1:A:220:PRO:HD2	2.16	0.59
1:A:24:LEU:HD13	1:A:26:LYS:CB	2.32	0.59
1:A:611:LEU:O	1:A:618:ALA:HB2	2.02	0.59
1:A:694:ASN:N	1:A:694:ASN:HD22	1.99	0.59
1:A:399:LEU:HG	1:A:401:GLY:N	2.16	0.59
1:A:25:PHE:HA	1:A:704:ARG:NH2	2.18	0.59
1:A:289:THR:HB	1:A:291:GLU:OE1	2.03	0.58
1:A:409:LEU:HD22	1:A:413:LYS:HB3	1.84	0.58
1:A:706:TYR:CB	1:A:712:VAL:HG12	2.33	0.58
1:A:698:TYR:HE2	1:A:739:PHE:HE2	1.50	0.58
1:A:304:PHE:O	1:A:308:ASN:ND2	2.35	0.58
1:A:412:GLU:HG2	4:A:1375:HOH:O	2.02	0.58
1:A:499:ILE:HD11	1:A:745:PHE:CD1	2.39	0.58
1:A:585:LEU:O	1:A:589:LYS:HG3	2.03	0.57
1:A:213:GLN:O	1:A:217:GLN:HG2	2.04	0.57
1:A:619:SER:CB	1:A:627:PHE:HE2	2.14	0.57
1:A:276:ARG:NH1	1:A:282:TYR:CG	2.72	0.57
1:A:534:VAL:HG22	1:A:535:PHE:CE2	2.39	0.57
1:A:685:ILE:HG22	1:A:686:ARG:N	2.18	0.57
1:A:509:ASP:O	4:A:1254:HOH:O	2.18	0.57
1:A:589:LYS:HB2	1:A:591:PRO:HD3	1.87	0.57
1:A:709:ALA:HB1	1:A:729:HIS:CE1	2.39	0.56
1:A:26:LYS:O	1:A:29:VAL:HG22	2.05	0.56
1:A:534:VAL:CG2	1:A:535:PHE:CE2	2.88	0.56
1:A:375:LEU:HD23	1:A:375:LEU:C	2.25	0.56
1:A:465:SER:OG	1:A:587:LYS:NZ	2.38	0.56
1:A:686:ARG:HA	1:A:689:ARG:CB	2.36	0.56
1:A:358:LYS:NZ	4:A:1236:HOH:O	2.39	0.56
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.10	0.56
1:A:725:ALA:O	1:A:728:LYS:N	2.39	0.56
1:A:99:GLU:H	1:A:100:PRO:CD	2.18	0.55
1:A:492:GLU:O	1:A:495:LEU:HB2	2.06	0.55
1:A:698:TYR:OH	1:A:739:PHE:HD2	1.90	0.55
1:A:43:GLU:CB	1:A:670:LYS:HZ2	2.18	0.55
1:A:621:ALA:HB2	1:A:628:ILE:CG1	2.36	0.55
1:A:380:THR:CG2	1:A:381:VAL:N	2.68	0.55
1:A:234:ASN:ND2	4:A:1220:HOH:O	2.40	0.55
1:A:705:TYR:O	1:A:726:VAL:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ALA:O	1:A:381:VAL:HG22	2.07	0.54
1:A:721:LYS:O	1:A:724:ASP:HB2	2.07	0.54
1:A:486:MET:CE	1:A:687:ILE:HG21	2.37	0.54
1:A:719:SER:O	1:A:722:ALA:N	2.41	0.54
1:A:704:ARG:HB3	1:A:705:TYR:CE2	2.42	0.54
1:A:223:GLU:O	1:A:227:ASN:HB2	2.07	0.54
1:A:324:PHE:CE2	1:A:328:ARG:HD2	2.43	0.54
1:A:480:GLN:HG3	1:A:508:LEU:HD13	1.89	0.54
1:A:594:GLN:NE2	1:A:594:GLN:HA	2.17	0.53
1:A:688:THR:O	1:A:691:GLY:N	2.40	0.53
1:A:443:GLN:HG2	1:A:446:LYS:HB3	1.90	0.53
1:A:292:GLU:O	1:A:295:ALA:HB3	2.09	0.53
1:A:296:LEU:O	1:A:297:HIS:HB2	2.09	0.53
1:A:380:THR:HG23	1:A:381:VAL:HG13	1.91	0.53
1:A:735:GLU:HB2	1:A:747:ARG:HH21	1.72	0.53
1:A:97:LEU:O	1:A:98:ASN:O	2.27	0.53
1:A:24:LEU:HB3	1:A:26:LYS:H	1.74	0.53
1:A:63:LYS:HG3	1:A:68:GLN:O	2.09	0.53
1:A:695:ARG:CB	1:A:745:PHE:CE2	2.92	0.53
1:A:45:ASP:CG	1:A:677:ARG:HH22	2.13	0.52
1:A:693:PRO:HD2	1:A:746:PHE:O	2.09	0.52
1:A:26:LYS:HA	1:A:29:VAL:HG13	1.90	0.52
1:A:98:ASN:O	1:A:102:VAL:HG23	2.09	0.52
1:A:344:ILE:O	1:A:348:ILE:HG12	2.10	0.52
1:A:513:THR:O	1:A:517:ILE:HD12	2.10	0.52
1:A:219:ASN:N	1:A:220:PRO:CD	2.73	0.52
1:A:319:SER:OG	1:A:322:GLU:HB2	2.10	0.52
1:A:694:ASN:ND2	1:A:694:ASN:H	2.05	0.52
1:A:99:GLU:N	1:A:100:PRO:CD	2.72	0.52
1:A:4:ILE:CD1	1:A:4:ILE:N	2.72	0.51
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.75	0.51
1:A:379:SER:HA	1:A:384:VAL:HG23	1.93	0.51
1:A:99:GLU:HG2	1:A:682:LEU:HD13	1.91	0.51
1:A:653:VAL:C	1:A:654:ARG:HE	2.14	0.51
1:A:99:GLU:H	1:A:100:PRO:HD2	1.75	0.51
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.93	0.51
1:A:437:ILE:O	1:A:441:LEU:HG	2.11	0.51
1:A:43:GLU:HG3	1:A:43:GLU:O	2.12	0.50
1:A:408:HIS:HD2	1:A:409:LEU:N	2.09	0.50
1:A:692:PHE:CZ	1:A:747:ARG:NH1	2.80	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.46	0.50

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ALA:N	1:A:291:GLU:OE2	2.45	0.50
1:A:354:LEU:O	1:A:418:ARG:HD3	2.12	0.50
1:A:696:ILE:O	1:A:743:LYS:HA	2.12	0.50
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.93	0.50
1:A:609:THR:CG2	1:A:613:ASN:ND2	2.75	0.50
1:A:710:PRO:O	1:A:711:ASN:OD1	2.30	0.50
1:A:367:ALA:O	1:A:408:HIS:NE2	2.44	0.49
1:A:458:PHE:CZ	1:A:573:TYR:HB3	2.47	0.49
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.93	0.49
1:A:147:ARG:NH1	4:A:1215:HOH:O	2.23	0.49
1:A:102:VAL:HG21	1:A:685:ILE:HD13	1.95	0.49
1:A:737:TYR:HB3	1:A:746:PHE:HE1	1.70	0.49
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.47	0.49
1:A:280:ILE:HD11	1:A:345:PHE:HE1	1.77	0.49
1:A:594:GLN:O	1:A:597:GLU:HB2	2.12	0.49
1:A:582:GLN:NE2	4:A:1245:HOH:O	2.27	0.49
1:A:753:ARG:NH1	1:A:753:ARG:HG3	2.27	0.49
1:A:621:ALA:CB	1:A:628:ILE:HG12	2.37	0.49
1:A:28:THR:HG21	1:A:84:LYS:HB2	1.96	0.48
1:A:594:GLN:NE2	1:A:594:GLN:CA	2.74	0.48
1:A:470:CYS:HB3	1:A:634:TYR:CZ	2.48	0.48
1:A:738:ARG:HB3	1:A:745:PHE:HB2	1.95	0.48
1:A:442:CYS:SG	1:A:443:GLN:N	2.86	0.48
1:A:609:THR:HG23	1:A:613:ASN:ND2	2.28	0.48
1:A:85:PHE:O	1:A:88:VAL:HG13	2.14	0.48
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.49	0.48
1:A:191:LYS:NZ	4:A:1365:HOH:O	2.25	0.48
1:A:286:ALA:HB1	1:A:321:SER:OG	2.13	0.48
1:A:428:ARG:O	1:A:431:LEU:HB2	2.14	0.48
1:A:99:GLU:N	1:A:100:PRO:HD2	2.29	0.48
1:A:331:MET:CE	1:A:345:PHE:CZ	2.96	0.48
1:A:723:THR:CG2	1:A:739:PHE:CZ	2.91	0.48
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.97	0.48
1:A:702:VAL:O	1:A:706:TYR:HB3	2.14	0.48
1:A:722:ALA:O	1:A:725:ALA:HB3	2.13	0.48
1:A:96:TYR:CE2	1:A:749:GLY:HA2	2.49	0.47
1:A:217:GLN:HG3	1:A:333:ILE:HD13	1.95	0.47
1:A:701:PHE:O	1:A:705:TYR:HD2	1.97	0.47
1:A:84:LYS:HD2	1:A:755:GLU:OE2	2.15	0.47
1:A:24:LEU:CD1	1:A:26:LYS:CB	2.92	0.47
1:A:499:ILE:CD1	1:A:745:PHE:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HB1	1:A:292:GLU:HB2	1.97	0.47
1:A:311:GLY:N	4:A:1144:HOH:O	2.36	0.47
1:A:680:GLY:N	4:A:1099:HOH:O	2.45	0.47
1:A:324:PHE:O	1:A:328:ARG:HG3	2.15	0.47
1:A:217:GLN:HG3	1:A:333:ILE:CD1	2.45	0.47
1:A:695:ARG:CB	1:A:745:PHE:CD2	2.98	0.47
1:A:683:GLU:HG3	1:A:686:ARG:NH2	2.30	0.47
1:A:614:ASP:O	1:A:616:ASN:N	2.48	0.46
1:A:96:TYR:CE2	1:A:749:GLY:CA	2.97	0.46
1:A:31:ASP:O	1:A:32:LYS:HG2	2.14	0.46
1:A:696:ILE:O	1:A:743:LYS:CA	2.64	0.46
1:A:297:HIS:O	1:A:298:LEU:HD23	2.15	0.46
1:A:371:ASP:OD2	1:A:372:LYS:N	2.48	0.46
1:A:218:ALA:C	1:A:220:PRO:HD2	2.36	0.46
1:A:643:ALA:O	1:A:647:THR:HG23	2.15	0.46
1:A:176:LEU:HD12	1:A:176:LEU:N	2.31	0.46
1:A:219:ASN:ND2	4:A:1426:HOH:O	2.38	0.46
1:A:296:LEU:O	1:A:298:LEU:HD23	2.16	0.46
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.30	0.46
1:A:567:GLU:HA	1:A:579:TYR:O	2.15	0.46
1:A:582:GLN:H	1:A:582:GLN:CD	2.16	0.46
1:A:219:ASN:HD21	1:A:243:ILE:HD11	1.80	0.46
1:A:726:VAL:HG12	1:A:730:LEU:CD1	2.45	0.46
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.98	0.46
1:A:735:GLU:CB	1:A:747:ARG:NH2	2.68	0.46
1:A:6:ASP:O	1:A:8:THR:N	2.48	0.46
1:A:340:GLU:O	1:A:344:ILE:HG13	2.16	0.46
1:A:59:SER:CB	1:A:72:VAL:O	2.64	0.46
1:A:456:SER:OG	1:A:457:GLY:N	2.49	0.45
1:A:534:VAL:HG22	1:A:535:PHE:CD2	2.51	0.45
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.68	0.45
1:A:568:PHE:O	1:A:578:MET:HE3	2.17	0.45
1:A:495:LEU:N	1:A:495:LEU:CD1	2.79	0.45
1:A:686:ARG:CB	1:A:689:ARG:CZ	2.94	0.45
1:A:578:MET:HA	1:A:578:MET:HE3	1.98	0.45
1:A:654:ARG:NH1	4:A:1349:HOH:O	2.49	0.45
1:A:728:LYS:O	1:A:731:ASN:N	2.46	0.45
1:A:697:ILE:HD12	1:A:743:LYS:HG2	1.99	0.45
1:A:82:PRO:HG2	1:A:85:PHE:HE1	1.81	0.45
1:A:685:ILE:HG22	1:A:689:ARG:HH11	1.82	0.45
1:A:147:ARG:O	1:A:150:GLU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.82	0.45
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.51	0.45
1:A:590:ASP:N	1:A:591:PRO:CD	2.79	0.45
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.52	0.45
1:A:3:PRO:O	1:A:12:HIS:HD2	2.00	0.45
1:A:633:GLN:O	1:A:637:GLN:HG3	2.17	0.45
1:A:709:ALA:CB	1:A:729:HIS:ND1	2.68	0.45
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.16	0.45
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.30	0.44
1:A:38:ASN:N	1:A:38:ASN:HD22	2.15	0.44
1:A:497:GLU:C	1:A:741:ILE:HD12	2.38	0.44
1:A:222:LEU:CD1	1:A:258:ILE:HD13	2.47	0.44
1:A:521:GLN:HA	1:A:522:PRO:C	2.38	0.44
1:A:415:SER:O	1:A:418:ARG:HB3	2.16	0.44
1:A:120:GLY:O	1:A:148:ARG:NH2	2.46	0.44
1:A:493:GLU:C	1:A:495:LEU:N	2.68	0.44
1:A:2:ASN:ND2	4:A:1196:HOH:O	2.51	0.44
1:A:4:ILE:HD12	1:A:4:ILE:N	2.32	0.44
1:A:696:ILE:O	1:A:744:ILE:N	2.45	0.44
1:A:289:THR:C	1:A:291:GLU:N	2.69	0.43
1:A:297:HIS:N	1:A:297:HIS:ND1	2.66	0.43
1:A:375:LEU:HD22	1:A:386:PRO:HB3	2.00	0.43
1:A:424:ALA:O	1:A:428:ARG:HG3	2.18	0.43
1:A:605:ASP:OD1	1:A:607:VAL:N	2.49	0.43
1:A:723:THR:CG2	1:A:739:PHE:CE2	3.00	0.43
1:A:359:PHE:HB3	1:A:411:VAL:HG12	1.99	0.43
1:A:462:LYS:HG3	4:A:1243:HOH:O	2.17	0.43
1:A:686:ARG:HB3	1:A:689:ARG:CZ	2.49	0.43
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.17	0.43
1:A:351:ILE:HG23	1:A:422:VAL:HG13	2.01	0.43
1:A:686:ARG:HB3	1:A:689:ARG:NH2	2.33	0.43
1:A:692:PHE:HB3	1:A:745:PHE:HB3	2.00	0.43
1:A:375:LEU:HD23	1:A:375:LEU:O	2.19	0.43
1:A:488:LYS:C	1:A:490:GLU:H	2.21	0.43
1:A:698:TYR:CD2	1:A:720:GLN:HA	2.54	0.43
1:A:341:GLN:O	1:A:345:PHE:CD2	2.72	0.43
1:A:499:ILE:HG22	1:A:500:ASN:H	1.84	0.43
1:A:369:LEU:O	1:A:372:LYS:NZ	2.45	0.43
1:A:493:GLU:C	1:A:495:LEU:H	2.20	0.43
1:A:614:ASP:C	1:A:616:ASN:N	2.72	0.43
1:A:609:THR:O	1:A:613:ASN:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:HB2	1:A:78:ASN:HB3	2.00	0.43
1:A:535:PHE:CD2	1:A:535:PHE:N	2.86	0.43
1:A:670:LYS:HG3	4:A:1199:HOH:O	2.19	0.43
1:A:49:CYS:SG	1:A:80:ARG:HD2	2.59	0.43
1:A:532:GLN:NE2	1:A:542:THR:OG1	2.47	0.42
1:A:698:TYR:CE2	1:A:739:PHE:CE2	3.04	0.42
1:A:614:ASP:C	1:A:616:ASN:H	2.21	0.42
1:A:697:ILE:HG22	1:A:700:ASP:N	2.31	0.42
1:A:707:LEU:C	1:A:709:ALA:H	2.22	0.42
1:A:590:ASP:N	1:A:591:PRO:HD3	2.34	0.42
1:A:368:VAL:HG22	1:A:369:LEU:N	2.35	0.42
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.54	0.42
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.20	0.42
1:A:281:PHE:O	1:A:285:LEU:HG	2.20	0.42
1:A:326:ILE:O	1:A:329:GLN:HB2	2.19	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.49	0.42
1:A:443:GLN:CG	1:A:445:ARG:C	2.75	0.42
1:A:701:PHE:O	1:A:705:TYR:N	2.53	0.42
1:A:169:ASP:C	1:A:170:ARG:HG2	2.40	0.42
1:A:265:LYS:HD3	1:A:427:GLY:HA3	2.01	0.42
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.79	0.42
1:A:181:SER:HA	3:A:999:DAE:F1	2.10	0.42
1:A:112:GLN:O	1:A:113:ASP:HB2	2.19	0.42
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.85	0.42
1:A:477:LYS:NZ	4:A:1093:HOH:O	2.46	0.42
1:A:628:ILE:HG21	1:A:628:ILE:HD13	1.86	0.42
1:A:7:ARG:NH1	1:A:19:GLN:OE1	2.53	0.42
1:A:319:SER:OG	1:A:322:GLU:CB	2.68	0.41
1:A:493:GLU:O	1:A:496:LYS:HB2	2.19	0.41
1:A:685:ILE:HG22	1:A:689:ARG:NH1	2.35	0.41
1:A:96:TYR:HE2	1:A:749:GLY:HA3	1.85	0.41
1:A:96:TYR:CE2	1:A:749:GLY:HA3	2.55	0.41
1:A:43:GLU:HA	1:A:670:LYS:NZ	2.33	0.41
1:A:488:LYS:HB2	1:A:488:LYS:HE2	1.83	0.41
1:A:593:GLN:HB2	1:A:596:LEU:HD12	2.02	0.41
1:A:698:TYR:CE2	1:A:739:PHE:HE2	2.34	0.41
1:A:43:GLU:CB	1:A:670:LYS:NZ	2.79	0.41
1:A:289:THR:C	1:A:291:GLU:H	2.24	0.41
1:A:488:LYS:C	1:A:490:GLU:N	2.73	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.86	0.41
1:A:609:THR:O	1:A:613:ASN:ND2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:O	1:A:216:LEU:HG	2.21	0.41
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.55	0.41
1:A:193:ILE:HG21	1:A:193:ILE:HD13	1.81	0.41
1:A:397:ARG:HB3	1:A:404:LEU:HG	2.03	0.41
1:A:581:ILE:N	1:A:582:GLN:OE1	2.54	0.41
1:A:593:GLN:O	1:A:596:LEU:HB2	2.20	0.41
1:A:34:TYR:HB2	1:A:51:GLU:HA	2.00	0.41
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.85	0.41
1:A:323:GLU:O	1:A:326:ILE:HB	2.21	0.41
1:A:680:GLY:CA	4:A:1099:HOH:O	2.68	0.41
1:A:676:LEU:HB3	1:A:682:LEU:HG	2.03	0.41
3:A:999:DAE:HA21	3:A:999:DAE:H6	1.62	0.41
1:A:202:ARG:N	1:A:212:GLU:OE2	2.51	0.41
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.53	0.41
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.82	0.41
1:A:497:GLU:O	1:A:741:ILE:HB	2.20	0.41
1:A:686:ARG:CB	1:A:689:ARG:NH2	2.84	0.41
1:A:703:LYS:O	1:A:706:TYR:HD2	2.04	0.41
1:A:293:LYS:HA	1:A:298:LEU:HB2	2.02	0.41
1:A:204:GLN:H	1:A:204:GLN:HG3	1.72	0.40
1:A:280:ILE:O	1:A:280:ILE:HG13	2.21	0.40
1:A:399:LEU:HA	1:A:403:ASP:O	2.21	0.40
1:A:683:GLU:CG	1:A:686:ARG:NH2	2.84	0.40
1:A:727:LEU:O	1:A:731:ASN:N	2.54	0.40
1:A:339:GLU:CD	1:A:339:GLU:N	2.75	0.40
1:A:341:GLN:O	1:A:345:PHE:HD2	2.04	0.40
1:A:710:PRO:HD2	1:A:729:HIS:CG	2.56	0.40
1:A:10:ASP:O	1:A:13:LYS:HB3	2.21	0.40
1:A:212:GLU:O	1:A:216:LEU:HD12	2.22	0.40
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.40
1:A:378:ALA:O	1:A:381:VAL:HG22	2.22	0.40
1:A:379:SER:HB3	1:A:384:VAL:O	2.21	0.40
1:A:600:PHE:HB3	1:A:612:PHE:CE1	2.56	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	737/761 (97%)	654 (89%)	62 (8%)	21 (3%)	6 2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	714	ARG
1	A	741	ILE
1	A	7	ARG
1	A	29	VAL
1	A	60	PHE
1	A	68	GLN
1	A	293	LYS
1	A	498	LYS
1	A	719	SER
1	A	386	PRO
1	A	693	PRO
1	A	711	ASN
1	A	713	PRO
1	A	725	ALA
1	A	86	ASP
1	A	718	ASP
1	A	754	ILE
1	A	703	LYS
1	A	362	GLY
1	A	3	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	594/665 (89%)	536 (90%)	58 (10%)	9	5

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	ILE
1	A	22	SER
1	A	28	THR
1	A	29	VAL
1	A	38	ASN
1	A	40	ASP
1	A	46	SER
1	A	56	THR
1	A	66	ASP
1	A	74	LYS
1	A	75	ASP
1	A	84	LYS
1	A	91	MET
1	A	98	ASN
1	A	130	LYS
1	A	147	ARG
1	A	148	ARG
1	A	158	ILE
1	A	204	GLN
1	A	266	SER
1	A	291	GLU
1	A	301	PRO
1	A	303	SER
1	A	307	LEU
1	A	319	SER
1	A	337	SER
1	A	369	LEU
1	A	388	VAL
1	A	389	LEU
1	A	391	LYS
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	444	GLU

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Mol	Chain	Res	Type
1	A	446	LYS
1	A	496	LYS
1	A	499	ILE
1	A	520	ARG
1	A	534	VAL
1	A	561	PRO
1	A	578	MET
1	A	594	GLN
1	A	636	GLU
1	A	654	ARG
1	A	683	GLU
1	A	687	ILE
1	A	688	THR
1	A	694	ASN
1	A	710	PRO
1	A	724	ASP
1	A	726	VAL
1	A	727	LEU
1	A	733	ASP
1	A	735	GLU
1	A	738	ARG
1	A	753	ARG
1	A	755	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	188	ASN
1	A	219	ASN
1	A	234	ASN
1	A	259	GLN
1	A	283	GLN
1	A	329	GLN
1	A	407	GLN
1	A	439	ASN
1	A	479	GLN
1	A	532	GLN
1	A	594	GLN
1	A	613	ASN
1	A	694	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	DAE	A	999	2	22,28,28	1.09	3 (13%)	24,42,42	1.69	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAE	A	999	2	-	0/21/28/28	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAE	C4-N4	2.10	1.49	1.46
3	A	999	DAE	C2-N2	2.52	1.50	1.46
3	A	999	DAE	C1-NA3	2.74	1.45	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	DAE	CA2-NA3-C1	-3.64	113.89	123.25
3	A	999	DAE	C5-C4-N4	2.43	121.28	119.38
3	A	999	DAE	C3-C2-N2	3.08	119.39	115.82
3	A	999	DAE	O4B-N4-C4	4.52	122.21	114.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	DAE	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	745/761 (97%)	1.45	185 (24%)	1	1	17, 46, 97, 100	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	11.5
1	A	494	TYR	10.6
1	A	27	LEU	10.0
1	A	744	ILE	9.2
1	A	712	VAL	8.7
1	A	24	LEU	8.3
1	A	498	LYS	8.0
1	A	716	ALA	8.0
1	A	710	PRO	7.9
1	A	25	PHE	7.7
1	A	713	PRO	7.7
1	A	362	GLY	7.4
1	A	65	VAL	7.0
1	A	500	ASN	6.9
1	A	443	GLN	6.8
1	A	495	LEU	6.7
1	A	497	GLU	6.5
1	A	745	PHE	6.5
1	A	715	ASP	6.3
1	A	536	PRO	6.2
1	A	706	TYR	6.2
1	A	725	ALA	6.1
1	A	31	ASP	6.1
1	A	492	GLU	6.1
1	A	698	TYR	6.1
1	A	718	ASP	6.0
1	A	501	TRP	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	6.0
1	A	702	VAL	6.0
1	A	723	THR	6.0
1	A	537	ASN	5.8
1	A	708	LEU	5.6
1	A	53	VAL	5.6
1	A	67	GLY	5.5
1	A	757	ALA	5.5
1	A	499	ILE	5.4
1	A	707	LEU	5.4
1	A	66	ASP	5.3
1	A	23	ASP	5.3
1	A	705	TYR	5.2
1	A	701	PHE	5.2
1	A	348	ILE	5.2
1	A	727	LEU	5.2
1	A	730	LEU	5.2
1	A	29	VAL	5.2
1	A	714	ARG	5.2
1	A	729	HIS	5.1
1	A	711	ASN	5.1
1	A	699	ALA	5.1
1	A	429	LEU	5.0
1	A	68	GLN	4.9
1	A	507	GLY	4.9
1	A	30	SER	4.9
1	A	738	ARG	4.8
1	A	743	LYS	4.8
1	A	722	ALA	4.8
1	A	491	GLN	4.7
1	A	742	THR	4.7
1	A	496	LYS	4.7
1	A	202	ARG	4.6
1	A	693	PRO	4.6
1	A	444	GLU	4.6
1	A	709	ALA	4.5
1	A	748	ALA	4.5
1	A	26	LYS	4.5
1	A	734	PRO	4.5
1	A	746	PHE	4.5
1	A	704	ARG	4.4
1	A	39	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	59	SER	4.2
1	A	700	ASP	4.0
1	A	401	GLY	4.0
1	A	697	ILE	3.9
1	A	732	ILE	3.9
1	A	740	GLY	3.9
1	A	717	GLU	3.8
1	A	733	ASP	3.8
1	A	3	PRO	3.8
1	A	366	GLY	3.8
1	A	296	LEU	3.7
1	A	426	TYR	3.7
1	A	62	PHE	3.7
1	A	692	PHE	3.7
1	A	721	LYS	3.7
1	A	352	LEU	3.7
1	A	758	ARG	3.7
1	A	225	PHE	3.7
1	A	728	LYS	3.6
1	A	2	ASN	3.6
1	A	5	HIS	3.6
1	A	689	ARG	3.6
1	A	430	PHE	3.6
1	A	615	PRO	3.6
1	A	759	GLU	3.6
1	A	719	SER	3.6
1	A	40	ASP	3.5
1	A	361	LYS	3.5
1	A	720	GLN	3.5
1	A	4	ILE	3.5
1	A	756	GLU	3.4
1	A	291	GLU	3.4
1	A	506	PHE	3.4
1	A	351	ILE	3.3
1	A	405	VAL	3.3
1	A	363	ALA	3.3
1	A	72	VAL	3.3
1	A	61	THR	3.2
1	A	28	THR	3.2
1	A	63	LYS	3.2
1	A	452	VAL	3.2
1	A	76	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	34	TYR	3.2
1	A	686	ARG	3.1
1	A	735	GLU	3.1
1	A	289	THR	3.1
1	A	274	THR	3.1
1	A	43	GLU	3.0
1	A	64	THR	3.0
1	A	726	VAL	3.0
1	A	493	GLU	3.0
1	A	124	VAL	3.0
1	A	739	PHE	3.0
1	A	724	ASP	3.0
1	A	281	PHE	2.9
1	A	21	ASP	2.9
1	A	123	LEU	2.9
1	A	175	LEU	2.9
1	A	425	LEU	2.9
1	A	45	ASP	2.9
1	A	335	GLY	2.9
1	A	747	ARG	2.9
1	A	421	LEU	2.9
1	A	736	GLN	2.8
1	A	489	LEU	2.8
1	A	754	ILE	2.8
1	A	290	ALA	2.8
1	A	280	ILE	2.8
1	A	399	LEU	2.8
1	A	751	LEU	2.8
1	A	38	ASN	2.7
1	A	52	ILE	2.7
1	A	364	GLY	2.7
1	A	755	GLU	2.7
1	A	753	ARG	2.7
1	A	731	ASN	2.7
1	A	422	VAL	2.7
1	A	339	GLU	2.7
1	A	243	ILE	2.6
1	A	60	PHE	2.6
1	A	204	GLN	2.6
1	A	322	GLU	2.5
1	A	115	ILE	2.5
1	A	106	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	158	ILE	2.5
1	A	347	ILE	2.5
1	A	77	ALA	2.5
1	A	752	ALA	2.4
1	A	222	LEU	2.4
1	A	177	ILE	2.4
1	A	56	THR	2.3
1	A	411	VAL	2.3
1	A	33	ARG	2.3
1	A	321	SER	2.3
1	A	741	ILE	2.3
1	A	37	TYR	2.2
1	A	655	CYS	2.2
1	A	453	LEU	2.2
1	A	221	ILE	2.2
1	A	203	ASN	2.2
1	A	58	ASP	2.2
1	A	627	PHE	2.2
1	A	600	PHE	2.1
1	A	433	LEU	2.1
1	A	690	LYS	2.1
1	A	268	VAL	2.1
1	A	42	LYS	2.1
1	A	603	SER	2.1
1	A	525	ILE	2.1
1	A	694	ASN	2.1
1	A	367	ALA	2.0
1	A	618	ALA	2.0
1	A	108	VAL	2.0
1	A	192	VAL	2.0
1	A	653	VAL	2.0
1	A	239	PHE	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	DAE	A	999	28/28	0.96	0.16	0.72	19,54,100,100	0
2	MG	A	998	1/1	0.94	0.07	-4.55	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.