Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGJ
Title	:	CRYSTAL STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI, ASN201ALA VARIANT.
Authors	:	Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on	:	2000-08-21
Resolution	:	1.92 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:

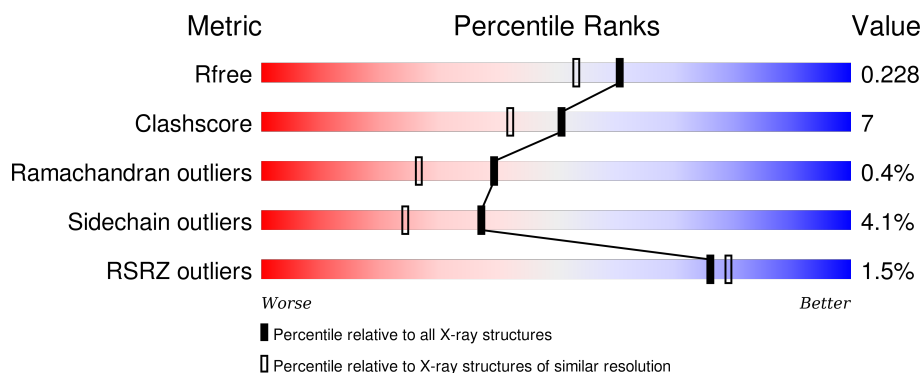|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.92 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
Rfree		0.228
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		4.1%
RSRZ outliers		1.5%

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))
R$_{free}$	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	753	% 81% 15% · ·
1	B	753	2% 78% 17% · ·
1	C	753	% 78% 17% · ·
1	D	753	% 78% 16% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25962 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.
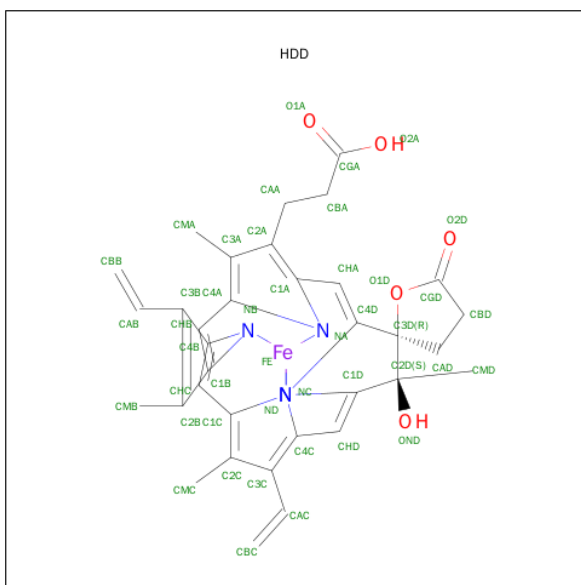
- Molecule 1 is a protein called CATALASE HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	B	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	C	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			
1	D	727	Total	C	N	O	S	0	0	0
			5743	3646	1004	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	ASN	ENGINEERED	UNP P21179
B	201	ALA	ASN	ENGINEERED	UNP P21179
C	201	ALA	ASN	ENGINEERED	UNP P21179
D	201	ALA	ASN	ENGINEERED	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	731	Total	O	0	0
			731	731		
3	B	655	Total	O	0	0
			655	655		
3	C	704	Total	O	0	0
			704	704		
3	D	724	Total	O	0	0
			724	724		

3 Residue-property plots ⓘ

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.
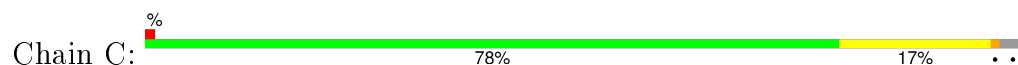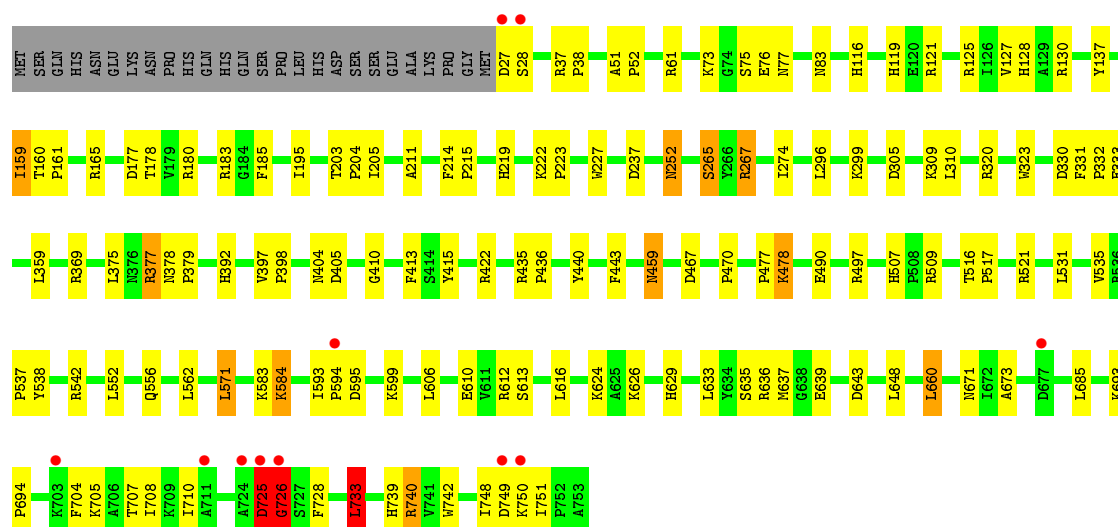
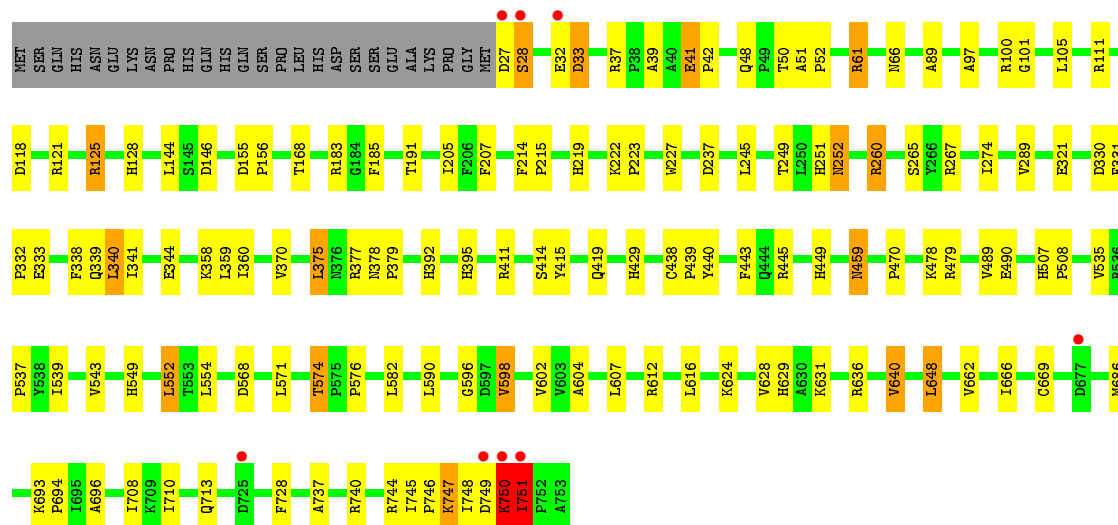• Molecule 1: CATALASE HPII
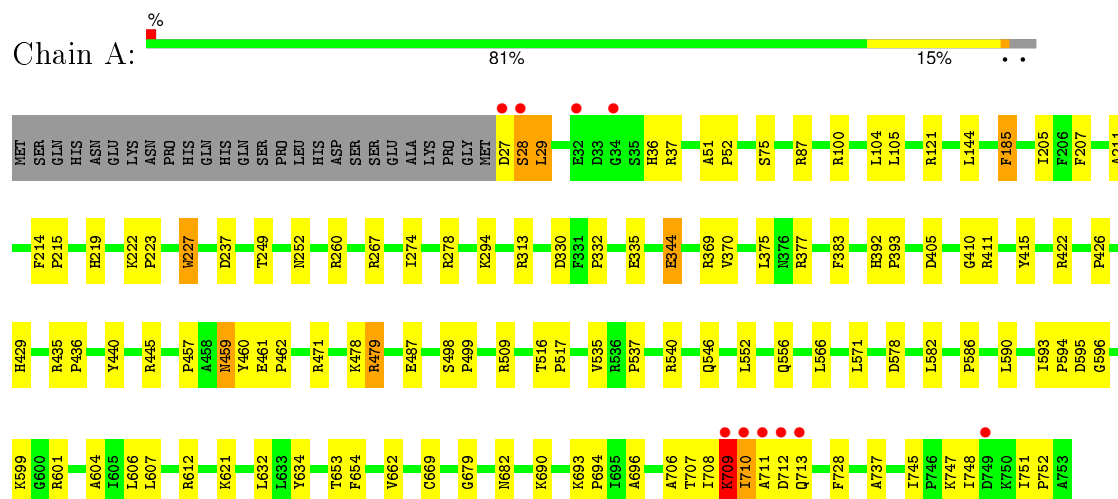
Chain A:

• Molecule 1: CATALASE HPII

Chain B:

• Molecule 1: CATALASE HPII

Chain C:

• Molecule 1: CATALASE HPII

Chain D:
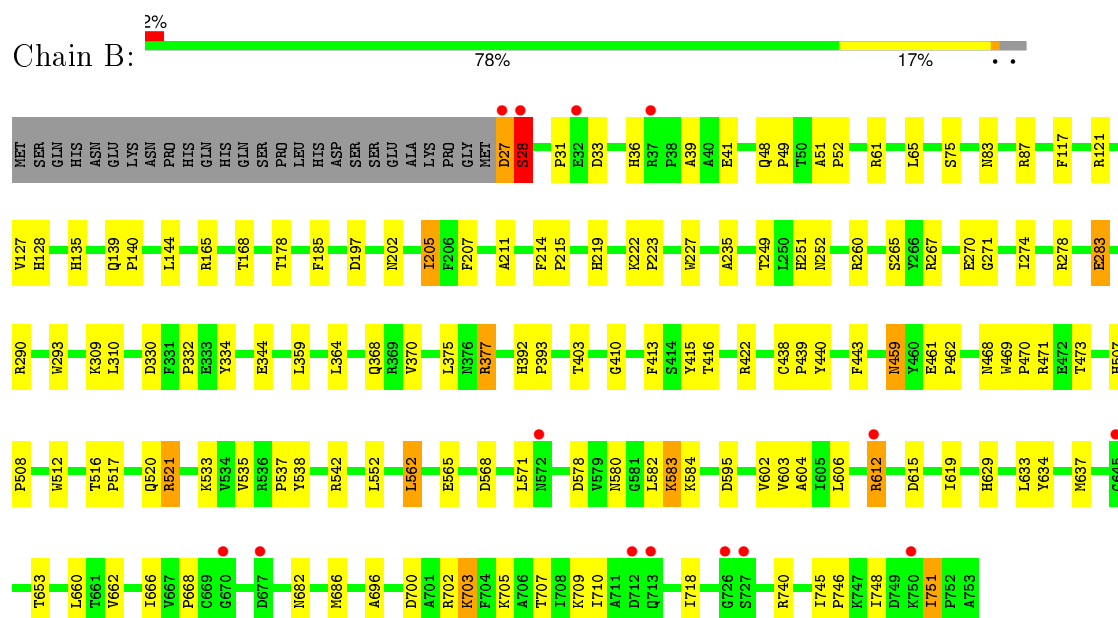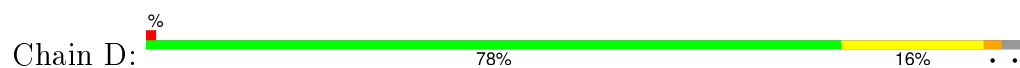
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.04Å　　132.34Å　　121.20Å 90.00°　　109.63°　　90.00°	Depositor
Resolution (Å)	87.71　–　1.92 19.26　–　1.92	Depositor EDS
% Data completeness (in resolution range)	91.7 (87.71-1.92) 91.7 (19.26-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182　,　0.235 0.181　,　0.228	Depositor DCC
R_{free} test set	9696 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	7.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.4	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 193708 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25962	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HDD

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	0.43	0/5899	1.11	24/8020 (0.3%)
1	B	0.43	0/5899	1.11	21/8020 (0.3%)
1	C	0.43	0/5899	1.10	19/8020 (0.2%)
1	D	0.42	0/5899	1.14	24/8020 (0.3%)
All	All	0.43	0/23596	1.11	88/32080 (0.3%)

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	C	0	1

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	445	ARG	NE-CZ-NH1	18.13	129.37	120.30
1	B	521	ARG	CD-NE-CZ	13.33	142.27	123.60
1	B	377	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	A	445	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	D	61	ARG	NE-CZ-NH2	11.33	125.97	120.30
1	D	377	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	D	260	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	C	725	ASP	C-N-CA	10.37	144.07	122.30
1	D	445	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	C	165	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	D	100	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	A	479	ARG	NE-CZ-NH1	9.38	124.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	612	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	D	121	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	290	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	100	ARG	CD-NE-CZ	7.61	134.25	123.60
1	D	61	ARG	CD-NE-CZ	7.59	134.23	123.60
1	C	422	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	B	283	GLU	CA-CB-CG	7.41	129.71	113.40
1	C	725	ASP	CA-C-O	7.41	135.65	120.10
1	A	509	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	D	61	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	C	467	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	540	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	125	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	497	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	180	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	377	ARG	CD-NE-CZ	7.05	133.48	123.60
1	A	100	ARG	CD-NE-CZ	7.04	133.46	123.60
1	C	740	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	521	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	C	177	ASP	CB-CG-OD2	6.88	124.49	118.30
1	C	509	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	D	479	ARG	CD-NE-CZ	6.74	133.03	123.60
1	B	278	ARG	CD-NE-CZ	6.72	133.01	123.60
1	B	87	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	61	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	C	726	GLY	N-CA-C	-6.49	96.87	113.10
1	B	165	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	377	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	D	445	ARG	CD-NE-CZ	6.39	132.55	123.60
1	A	377	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	612	ARG	CD-NE-CZ	6.36	132.50	123.60
1	A	422	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	422	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	180	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	636	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	377	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	383	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	313	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	A	479	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	121	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	509	ARG	NE-CZ-NH2	5.93	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	CD-NE-CZ	5.88	131.83	123.60
1	B	334	TYR	CB-CG-CD2	-5.79	117.52	121.00
1	A	471	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	D	121	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	479	ARG	CD-NE-CZ	5.74	131.63	123.60
1	A	445	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	260	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	130	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	449	HIS	CA-CB-CG	5.59	123.11	113.60
1	D	740	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	37	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	521	ARG	CA-CB-CG	5.55	125.60	113.40
1	D	183	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	87	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	D	125	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	552	LEU	CA-CB-CG	5.38	127.67	115.30
1	D	111	ARG	CD-NE-CZ	5.36	131.10	123.60
1	D	377	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	D	260	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	471	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	B	121	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	37	ARG	CD-NE-CZ	5.22	130.90	123.60
1	C	733	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	344	GLU	CA-CB-CG	5.13	124.70	113.40
1	A	601	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	28	SER	N-CA-CB	5.12	118.19	110.50
1	C	121	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	405	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	740	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	117	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	B	403	THR	N-CA-CB	5.05	119.89	110.30
1	C	320	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	D	118	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	A	185	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	Mainchain

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	5743	0	5577	72	0
1	B	5743	0	5577	80	0
1	C	5743	0	5576	81	0
1	D	5743	0	5577	86	0
2	A	44	0	31	7	0
2	B	44	0	31	5	0
2	C	44	0	31	5	0
2	D	44	0	31	4	0
3	A	731	0	0	6	0
3	B	655	0	0	4	0
3	C	704	0	0	13	0
3	D	724	0	0	10	0
All	All	25962	0	22431	309	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 7.

All (309) 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:392:HIS:ND1	1:B:415:TYR:HB2	1.13	1.42
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.12	1.38
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.09	1.38
1:A:392:HIS:ND1	1:A:415:TYR:HB2	1.09	1.37
2:B:760:HDD:HMC1	2:B:760:HDD:HBC1	1.33	1.07
1:C:274:ILE:HD12	2:C:760:HDD:HMB1	1.56	0.87
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.11	0.85
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.11	0.85
2:A:760:HDD:HMC1	2:A:760:HDD:HBC1	1.56	0.85
1:D:750:LYS:HD3	1:D:751:ILE:H	1.50	0.76
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.52	0.73
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.16	0.73
2:B:760:HDD:CMC	2:B:760:HDD:HBC1	2.13	0.72
1:B:267:ARG:HG3	3:B:1240:HOH:O	1.88	0.72
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.19	0.71
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.18	0.70
1:C:137:TYR:HB2	1:C:159:ILE:HD13	1.73	0.70
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.72	0.70
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.74	0.69
1:A:556:GLN:HG3	1:A:566:LEU:HD12	1.75	0.69
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.76	0.67
1:A:274:ILE:HD12	2:A:760:HDD:HMB1	1.77	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.76	0.66
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.77	0.66
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.77	0.66
1:B:583:LYS:O	1:B:584:LYS:HB3	1.93	0.65
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.78	0.65
2:A:760:HDD:HBB1	2:A:760:HDD:HMB1	1.78	0.64
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.80	0.64
2:A:760:HDD:HMC1	2:A:760:HDD:CBC	2.26	0.64
1:D:629:HIS:HD2	3:D:1117:HOH:O	1.81	0.64
1:B:468:ASN:HD22	1:D:27:ASP:N	1.96	0.64
1:A:546:GLN:HG3	3:A:1455:HOH:O	1.98	0.64
1:B:416:THR:HG21	3:D:1401:HOH:O	1.99	0.63
1:A:29:LEU:HB2	3:C:1365:HOH:O	1.98	0.63
1:C:267:ARG:HD3	3:C:1249:HOH:O	1.99	0.62
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.81	0.62
1:D:274:ILE:HD12	2:D:760:HDD:HMB1	1.80	0.62
1:C:624:LYS:HD3	3:C:1400:HOH:O	2.00	0.61
1:C:748:ILE:O	1:C:751:ILE:HG22	2.01	0.61
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.83	0.61
2:C:760:HDD:HBC1	2:C:760:HDD:HMC1	1.81	0.61
1:D:267:ARG:HG3	3:D:1241:HOH:O	2.01	0.60
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.83	0.60
1:B:583:LYS:CE	1:B:583:LYS:H	2.16	0.59
1:A:745:ILE:O	1:A:748:ILE:HG12	2.03	0.59
1:D:222:LYS:HB3	1:D:223:PRO:HD2	1.85	0.59
1:D:27:ASP:O	1:D:28:SER:HB2	2.02	0.59
1:D:321:GLU:HG3	3:D:1307:HOH:O	2.03	0.58
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.18	0.58
1:D:750:LYS:CD	1:D:751:ILE:H	2.17	0.58
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.84	0.57
1:D:32:GLU:O	1:D:33:ASP:HB3	2.04	0.57
1:A:52:PRO:HG3	3:C:1012:HOH:O	2.04	0.57
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.86	0.57
1:B:521:ARG:HH21	1:B:745:ILE:CG2	2.15	0.57
2:A:760:HDD:HBC1	2:A:760:HDD:CMC	2.29	0.57
1:B:274:ILE:HD12	2:B:760:HDD:HMB1	1.86	0.57
1:B:666:ILE:HG12	1:B:696:ALA:HB3	1.86	0.57
1:A:621:LYS:HE3	3:A:1486:HOH:O	2.04	0.57
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.86	0.56
1:B:83:ASN:HB3	1:D:429:HIS:CD2	2.40	0.56
3:B:955:HOH:O	1:D:52:PRO:HG3	2.05	0.56
1:A:751:ILE:O	1:A:751:ILE:HD12	2.05	0.56
1:A:708:ILE:O	1:A:710:ILE:HB	2.05	0.56
1:A:556:GLN:HG3	1:A:566:LEU:CD1	2.34	0.56
1:D:745:ILE:O	1:D:748:ILE:HG12	2.06	0.56
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.88	0.56
1:A:679:GLY:HA3	1:D:750:LYS:O	2.06	0.55
1:C:299:LYS:HE3	1:C:595:ASP:OD1	2.07	0.55
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.35	0.54
2:A:760:HDD:HBB1	2:A:760:HDD:CMB	2.37	0.54
1:B:606:LEU:O	1:B:668:PRO:HD2	2.08	0.54
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.89	0.54
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.89	0.54
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.43	0.53
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.44	0.53
1:B:507:HIS:N	1:B:508:PRO:HD2	2.23	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53
1:A:748:ILE:O	1:A:751:ILE:HG13	2.08	0.53
1:B:178:THR:HG21	1:B:310:LEU:HD23	1.90	0.52
1:C:435:ARG:HD3	3:C:1118:HOH:O	2.09	0.52
1:A:478:LYS:HG2	3:A:1246:HOH:O	2.09	0.52
1:B:583:LYS:HE2	1:B:583:LYS:H	1.75	0.52
1:A:28:SER:CB	1:D:245:LEU:HD22	2.40	0.52
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.91	0.52
1:C:629:HIS:HD2	3:C:1079:HOH:O	1.92	0.52
1:D:640:VAL:HG23	1:D:648:LEU:HB2	1.91	0.52
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.91	0.52
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.90	0.52
1:D:602:VAL:HG13	1:D:662:VAL:HA	1.90	0.52
1:A:706:ALA:O	1:A:709:LYS:HD2	2.10	0.51
1:C:613:SER:HB3	1:C:643:ASP:OD1	2.10	0.51
1:C:599:LYS:HE2	3:C:1054:HOH:O	2.10	0.51
1:C:265:SER:OG	1:C:267:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.92	0.51
1:B:469:TRP:CE3	1:B:471:ARG:HG3	2.45	0.51
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.91	0.51
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.91	0.51
1:D:32:GLU:O	1:D:33:ASP:CB	2.59	0.51
1:A:104:LEU:HB3	3:A:900:HOH:O	2.11	0.51
1:C:183:ARG:HG2	3:C:1294:HOH:O	2.10	0.51
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.92	0.50
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.46	0.50
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.93	0.50
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.47	0.50
1:C:751:ILE:HB	3:C:1357:HOH:O	2.10	0.50
1:C:535:VAL:O	1:C:537:PRO:HD3	2.11	0.50
1:C:584:LYS:HB2	1:C:584:LYS:HZ3	1.76	0.50
1:B:52:PRO:HG3	3:D:1050:HOH:O	2.11	0.50
1:C:556:GLN:NE2	3:C:1394:HOH:O	2.44	0.50
1:A:596:GLY:HA3	1:A:737:ALA:O	2.12	0.49
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.94	0.49
1:D:27:ASP:O	1:D:28:SER:CB	2.60	0.49
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.77	0.49
1:A:586:PRO:HB2	1:A:593:ILE:HD11	1.95	0.49
1:B:36:HIS:HD1	1:B:36:HIS:H	1.59	0.49
1:B:128:HIS:HA	1:B:168:THR:O	2.13	0.49
1:A:267:ARG:HG2	1:A:332:PRO:HB3	1.94	0.49
1:D:666:ILE:HG12	1:D:696:ALA:HB3	1.94	0.49
1:A:710:ILE:HD11	1:A:747:LYS:HB3	1.94	0.49
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.49
1:B:700:ASP:O	1:B:703:LYS:HD3	2.12	0.49
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.49
1:B:535:VAL:O	1:B:537:PRO:HD3	2.13	0.49
1:B:748:ILE:O	1:B:751:ILE:HG22	2.12	0.49
1:B:271:GLY:HA3	1:B:293:TRP:HB2	1.95	0.49
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.95	0.48
1:A:708:ILE:O	1:A:709:LYS:C	2.52	0.48
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.94	0.48
1:D:214:PHE:HB3	1:D:215:PRO:HD3	1.94	0.48
1:D:607:LEU:HD13	1:D:640:VAL:HG21	1.94	0.48
1:C:739:HIS:CD2	1:C:740:ARG:HG2	2.49	0.48
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.48
1:B:637:MET:HB2	1:C:562:LEU:HA	1.96	0.48
1:D:549:HIS:O	1:D:576:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.95	0.48
1:B:629:HIS:HD2	3:B:1022:HOH:O	1.95	0.48
1:C:490:GLU:HA	1:D:489:VAL:O	2.14	0.48
1:D:146:ASP:HB2	3:D:1382:HOH:O	2.14	0.47
1:C:305:ASP:O	1:C:309:LYS:HG3	2.15	0.47
1:B:507:HIS:N	1:B:508:PRO:CD	2.77	0.47
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.15	0.47
1:C:583:LYS:O	1:C:584:LYS:HB3	2.15	0.47
1:D:411:ARG:HG2	2:D:760:HDD:C2C	2.45	0.46
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.46
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.19	0.46
1:D:41:GLU:CD	1:D:42:PRO:HD2	2.35	0.46
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.45	0.46
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.46
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.97	0.46
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.51	0.46
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.43	0.46
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.31	0.46
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.80	0.46
1:D:535:VAL:O	1:D:537:PRO:HD3	2.14	0.46
1:B:602:VAL:HG22	1:B:629:HIS:HB2	1.98	0.46
1:D:37:ARG:HB3	3:D:1462:HOH:O	2.15	0.46
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.97	0.46
1:B:634:TYR:O	1:B:653:THR:HA	2.15	0.46
1:B:473:THR:O	1:D:89:ALA:HA	2.16	0.46
1:A:426:PRO:HB2	1:C:116:HIS:CD2	2.51	0.46
1:D:507:HIS:N	1:D:508:PRO:HD2	2.31	0.46
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.98	0.45
1:C:178:THR:HG21	1:C:310:LEU:HD23	1.97	0.45
1:D:574:THR:HG22	3:D:1165:HOH:O	2.15	0.45
1:B:139:GLN:HA	1:B:140:PRO:HD3	1.76	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.34	0.45
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.30	0.45
2:B:760:HDD:HBB1	2:B:760:HDD:HMB1	1.98	0.45
1:B:702:ARG:O	1:B:705:LYS:HD3	2.16	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.51	0.45
1:C:459:ASN:H	1:C:459:ASN:HD22	1.64	0.45
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.99	0.45
1:C:626:LYS:HG3	1:C:733:LEU:HG	1.98	0.45
1:D:341:ILE:HD11	1:D:360:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLN:NE2	3:A:1437:HOH:O	2.49	0.45
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.99	0.45
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.45
1:A:330:ASP:OD2	1:A:599:LYS:NZ	2.48	0.45
1:C:704:PHE:O	1:C:707:THR:HG22	2.18	0.45
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.73	0.45
2:C:760:HDD:HBD2	3:C:959:HOH:O	2.16	0.44
1:A:27:ASP:O	1:A:28:SER:C	2.55	0.44
1:A:516:THR:HB	1:A:517:PRO:HD2	1.98	0.44
1:A:708:ILE:O	1:A:710:ILE:N	2.51	0.44
1:C:516:THR:HB	1:C:517:PRO:HD2	1.99	0.44
1:A:227:TRP:CZ3	1:D:50:THR:HG21	2.52	0.44
1:C:636:ARG:NH2	1:C:639:GLU:O	2.50	0.44
1:D:39:ALA:H	1:D:48:GLN:NE2	2.16	0.44
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.84	0.44
1:A:105:LEU:HD11	1:C:413:PHE:HB2	1.98	0.44
1:D:97:ALA:O	1:D:101:GLY:HA3	2.18	0.44
1:A:36:HIS:H	1:A:36:HIS:CD2	2.36	0.44
1:C:127:VAL:O	1:C:128:HIS:HB2	2.18	0.44
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.48	0.44
1:D:289:VAL:HA	1:D:339:GLN:O	2.18	0.44
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.00	0.44
1:C:404:ASN:O	1:C:405:ASP:C	2.54	0.44
1:B:368:GLN:O	1:B:370:VAL:HG23	2.18	0.44
1:C:28:SER:HA	3:C:1439:HOH:O	2.18	0.43
1:C:705:LYS:HB3	1:C:710:ILE:HB	1.99	0.43
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.43
1:C:27:ASP:HB3	3:C:1391:HOH:O	2.17	0.43
1:B:205:ILE:HD13	1:B:205:ILE:H	1.83	0.43
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.01	0.43
1:C:538:TYR:O	1:C:542:ARG:HG3	2.19	0.43
1:A:752:PRO:HB2	1:D:686:MET:SD	2.58	0.43
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.34	0.43
1:B:443:PHE:CE2	1:B:470:PRO:HD2	2.53	0.43
1:D:748:ILE:O	1:D:751:ILE:HG22	2.17	0.43
1:D:507:HIS:N	1:D:508:PRO:CD	2.81	0.43
1:A:578:ASP:HB3	1:A:582:LEU:O	2.18	0.43
1:A:211:ALA:HB3	1:A:410:GLY:HA3	2.00	0.43
1:C:331:PHE:HA	1:C:332:PRO:HD3	1.84	0.43
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.43
1:C:397:VAL:HB	1:C:398:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CG	1:C:83:ASN:HB3	2.53	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.36	0.43
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.19	0.43
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.01	0.43
1:B:516:THR:HB	1:B:517:PRO:CD	2.49	0.43
1:A:535:VAL:O	1:A:537:PRO:HD3	2.19	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:B:207:PHE:O	1:B:249:THR:HA	2.19	0.42
1:D:267:ARG:NH1	1:D:321:GLU:OE2	2.50	0.42
1:A:260:ARG:HD3	1:A:590:LEU:HD21	2.00	0.42
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.42
2:C:760:HDD:CBC	2:C:760:HDD:HMC1	2.49	0.42
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.02	0.42
1:D:392:HIS:HB3	1:D:395:HIS:CE1	2.55	0.42
1:A:498:SER:HA	1:A:499:PRO:HD3	1.88	0.42
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.95	0.42
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
2:B:760:HDD:HBB1	2:B:760:HDD:CMB	2.49	0.42
1:C:125:ARG:HB3	2:C:760:HDD:HBD1	2.01	0.42
1:D:155:ASP:HA	1:D:156:PRO:HD2	1.90	0.42
1:D:125:ARG:HB3	2:D:760:HDD:HBD1	2.02	0.42
1:D:332:PRO:HD2	1:D:375:LEU:O	2.20	0.42
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.42
1:C:740:ARG:HB2	1:C:742:TRP:CH2	2.54	0.42
1:B:27:ASP:HB3	3:B:1386:HOH:O	2.19	0.42
1:A:606:LEU:HD22	1:A:654:PHE:CE2	2.55	0.42
1:D:438:CYS:HB2	1:D:439:PRO:HD2	2.00	0.42
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.83	0.42
1:D:669:CYS:SG	3:D:1450:HOH:O	2.45	0.42
1:D:745:ILE:N	1:D:746:PRO:HD2	2.34	0.42
1:A:144:LEU:HD11	1:A:370:VAL:HG13	2.01	0.42
1:A:479:ARG:NH2	3:A:1449:HOH:O	2.47	0.42
1:D:539:ILE:O	1:D:543:VAL:HG23	2.20	0.42
1:D:415:TYR:O	1:D:419:GLN:OE1	2.37	0.41
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.41
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.33	0.41
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.01	0.41
1:A:435:ARG:HA	1:A:436:PRO:HD3	1.88	0.41
1:D:27:ASP:N	3:D:861:HOH:O	2.53	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:A:461:GLU:HB2	1:A:462:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PHE:HB3	1:B:215:PRO:HD3	2.03	0.41
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.68	0.41
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.01	0.41
1:C:214:PHE:N	1:C:215:PRO:CD	2.82	0.41
1:B:516:THR:HB	1:B:517:PRO:HD2	2.01	0.41
1:D:438:CYS:HB2	1:D:439:PRO:CD	2.51	0.41
1:A:552:LEU:HD21	1:A:571:LEU:O	2.19	0.41
1:B:461:GLU:HA	1:B:462:PRO:C	2.40	0.41
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.94	0.41
1:B:31:PRO:HB2	1:B:33:ASP:OD1	2.21	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.21	0.41
1:B:267:ARG:HD3	1:B:332:PRO:HG3	2.02	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.41
1:D:358:LYS:HD2	1:D:507:HIS:CE1	2.56	0.41
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.56	0.41
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.50	0.41
1:C:203:THR:HB	1:C:204:PRO:HD2	2.02	0.41
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.56	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.21	0.41
1:C:584:LYS:NZ	1:C:584:LYS:HB2	2.34	0.41
1:D:568:ASP:HA	1:D:571:LEU:HD12	2.02	0.41
1:B:39:ALA:HB1	1:B:41:GLU:HG2	2.03	0.41
1:B:413:PHE:HB2	1:D:105:LEU:HD11	2.02	0.41
1:D:744:ARG:O	1:D:748:ILE:HG23	2.21	0.41
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.41
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.56	0.41
1:A:426:PRO:HG3	1:C:119:HIS:HB2	2.02	0.41
1:D:260:ARG:HD3	1:D:590:LEU:HD21	2.02	0.41
1:D:331:PHE:O	1:D:333:GLU:HG3	2.20	0.41
1:B:344:GLU:H	1:B:344:GLU:CD	2.23	0.41
1:B:202:ASN:HA	1:B:270:GLU:O	2.21	0.41
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.69	0.41
1:C:323:TRP:CH2	1:C:378:ASN:HB3	2.56	0.40
1:D:596:GLY:HA3	1:D:737:ALA:O	2.21	0.40
1:B:512:TRP:CH2	1:B:520:GLN:HB3	2.57	0.40
1:C:160:THR:HA	1:C:161:PRO:HD3	1.96	0.40
1:D:624:LYS:C	1:D:624:LYS:HD3	2.41	0.40
1:B:615:ASP:O	1:B:619:ILE:HG13	2.20	0.40
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.02	0.40
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.67	0.40
1:C:159:ILE:C	1:C:159:ILE:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASP:HB3	1:B:582:LEU:O	2.21	0.40
1:D:414:SER:OG	2:D:760:HDD:HHD	2.21	0.40
1:D:378:ASN:HB3	1:D:379:PRO:HD2	2.03	0.40
1:B:197:ASP:HB2	1:B:392:HIS:O	2.22	0.40
1:A:411:ARG:HG2	2:A:760:HDD:C2C	2.52	0.40
1:B:538:TYR:O	1:B:542:ARG:HG3	2.21	0.40
1:D:128:HIS:HA	1:D:168:THR:O	2.21	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	725/753 (96%)	697 (96%)	24 (3%)	4 (1%)	30	16
1	B	725/753 (96%)	697 (96%)	26 (4%)	2 (0%)	46	34
1	C	725/753 (96%)	699 (96%)	23 (3%)	3 (0%)	39	27
1	D	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	30	16
All	All	2900/3012 (96%)	2793 (96%)	94 (3%)	13 (0%)	39	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	LYS
1	A	711	ALA
1	D	28	SER
1	D	751	ILE
1	A	28	SER
1	C	75	SER
1	C	725	ASP
1	D	33	ASP

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Mol	Chain	Res	Type
1	D	750	LYS
1	A	75	SER
1	B	28	SER
1	B	75	SER
1	C	726	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/635 (96%)	596 (98%)	15 (2%)	55	46
1	B	611/635 (96%)	587 (96%)	24 (4%)	39	26
1	C	611/635 (96%)	580 (95%)	31 (5%)	29	16
1	D	611/635 (96%)	582 (95%)	29 (5%)	32	19
All	All	2444/2540 (96%)	2345 (96%)	99 (4%)	37	24

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	294	LYS
1	A	344	GLU
1	A	375	LEU
1	A	440	TYR
1	A	459	ASN
1	A	595	ASP
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	B	27	ASP

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Mol	Chain	Res	Type
1	B	28	SER
1	B	127	VAL
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	265	SER
1	B	283	GLU
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	633	LEU
1	B	703	LYS
1	B	709	LYS
1	B	751	ILE
1	C	61	ARG
1	C	73	LYS
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	265	SER
1	C	267	ARG
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	521	ARG
1	C	531	LEU
1	C	571	LEU

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Mol	Chain	Res	Type
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	635	SER
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	733	LEU
1	C	749	ASP
1	C	750	LYS
1	D	41	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	265	SER
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	631	LYS
1	D	640	VAL
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	368	GLN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	368	GLN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS

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)

4 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	HDD	A	760	1,3	30,52,52	3.10	12 (40%)	20,89,89	3.48	9 (45%)
2	HDD	B	760	1,3	30,52,52	3.11	13 (43%)	20,89,89	3.69	10 (50%)
2	HDD	C	760	1,3	30,52,52	2.98	10 (33%)	20,89,89	4.00	12 (60%)
2	HDD	D	760	1	30,52,52	3.22	11 (36%)	20,89,89	3.22	11 (55%)

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
2	HDD	A	760	1,3	-	0/3/89/89	0/1/9/9
2	HDD	B	760	1,3	-	0/3/89/89	0/1/9/9
2	HDD	C	760	1,3	-	0/3/89/89	0/1/9/9
2	HDD	D	760	1	-	0/3/89/89	0/1/9/9

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	C2D-C3D	-11.01	1.27	1.54
2	C	760	HDD	C2D-C3D	-10.96	1.27	1.54
2	B	760	HDD	C2D-C3D	-10.95	1.27	1.54
2	A	760	HDD	C2D-C3D	-10.76	1.27	1.54
2	C	760	HDD	C3B-C2B	-4.17	1.34	1.40
2	B	760	HDD	C3B-C2B	-4.15	1.34	1.40
2	A	760	HDD	C3B-C2B	-3.91	1.35	1.40
2	A	760	HDD	C3C-C2C	-3.86	1.35	1.40
2	C	760	HDD	C3C-C2C	-3.61	1.35	1.40
2	D	760	HDD	C3C-C2C	-3.46	1.35	1.40
2	B	760	HDD	C3C-C2C	-3.43	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	O1D-CGD	-3.10	1.30	1.35
2	C	760	HDD	O1D-CGD	-3.06	1.30	1.35
2	D	760	HDD	C3B-C2B	-2.97	1.36	1.40
2	B	760	HDD	O1D-CGD	-2.96	1.30	1.35
2	A	760	HDD	O1D-CGD	-2.77	1.30	1.35
2	D	760	HDD	C4D-ND	-2.55	1.34	1.38
2	C	760	HDD	C4D-ND	-2.27	1.34	1.38
2	A	760	HDD	C4D-ND	-2.24	1.34	1.38
2	A	760	HDD	C1B-NB	-2.05	1.33	1.36
2	B	760	HDD	C4D-ND	-2.03	1.35	1.38
2	B	760	HDD	CMC-C2C	2.04	1.55	1.51
2	B	760	HDD	CMB-C2B	2.10	1.56	1.51
2	B	760	HDD	CAD-C3D	2.23	1.57	1.53
2	A	760	HDD	CMB-C2B	2.30	1.56	1.51
2	B	760	HDD	C3C-CAC	2.69	1.53	1.47
2	D	760	HDD	C3C-CAC	2.77	1.53	1.47
2	C	760	HDD	C3C-CAC	2.87	1.53	1.47
2	A	760	HDD	C3C-CAC	2.94	1.54	1.47
2	A	760	HDD	C3B-CAB	3.04	1.54	1.47
2	D	760	HDD	FE-ND	3.12	2.08	1.95
2	C	760	HDD	FE-ND	3.16	2.08	1.95
2	C	760	HDD	C3B-CAB	3.31	1.54	1.47
2	B	760	HDD	C3B-CAB	3.51	1.55	1.47
2	D	760	HDD	C3B-CAB	3.66	1.55	1.47
2	B	760	HDD	FE-ND	4.03	2.11	1.95
2	A	760	HDD	FE-ND	4.53	2.13	1.95
2	B	760	HDD	OND-C2D	4.78	1.52	1.42
2	C	760	HDD	OND-C2D	4.81	1.52	1.42
2	D	760	HDD	OND-C2D	4.86	1.52	1.42
2	A	760	HDD	OND-C2D	4.95	1.52	1.42
2	C	760	HDD	O1D-C3D	5.12	1.55	1.46
2	D	760	HDD	O1D-C3D	5.53	1.56	1.46
2	B	760	HDD	O1D-C3D	5.70	1.56	1.46
2	A	760	HDD	O1D-C3D	5.86	1.56	1.46
2	D	760	HDD	CAD-C3D	5.99	1.64	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HDD	OND-C2D-CMD	-11.04	89.48	109.41
2	A	760	HDD	OND-C2D-CMD	-6.40	97.86	109.41
2	A	760	HDD	CAA-C2A-C1A	-6.13	120.36	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HDD	C3C-CAC-CBC	-6.08	113.88	126.32
2	B	760	HDD	C3B-C4B-NB	-6.07	99.48	110.94
2	B	760	HDD	CAA-CBA-CGA	-6.00	101.75	112.75
2	A	760	HDD	C3B-C4B-NB	-5.97	99.68	110.94
2	B	760	HDD	C2D-C1D-CHD	-5.90	114.30	123.48
2	C	760	HDD	C3B-C4B-NB	-5.90	99.81	110.94
2	B	760	HDD	CAA-C2A-C1A	-5.85	120.66	127.01
2	B	760	HDD	C3C-CAC-CBC	-5.77	114.51	126.32
2	D	760	HDD	C3B-C4B-NB	-5.66	100.26	110.94
2	D	760	HDD	OND-C2D-CMD	-5.49	99.49	109.41
2	B	760	HDD	OND-C2D-CMD	-5.45	99.57	109.41
2	C	760	HDD	C2D-C1D-CHD	-5.41	115.05	123.48
2	D	760	HDD	C3C-CAC-CBC	-5.40	115.27	126.32
2	C	760	HDD	C3C-CAC-CBC	-5.17	115.74	126.32
2	C	760	HDD	CAA-C2A-C1A	-5.01	121.57	127.01
2	D	760	HDD	CAA-CBA-CGA	-4.93	103.71	112.75
2	A	760	HDD	O1D-CGD-CBD	-4.89	104.47	110.20
2	D	760	HDD	C2D-C1D-CHD	-4.57	116.36	123.48
2	D	760	HDD	CAA-C2A-C1A	-4.41	122.22	127.01
2	C	760	HDD	CAA-CBA-CGA	-4.30	104.86	112.75
2	B	760	HDD	C3B-CAB-CBB	-4.16	117.81	126.32
2	A	760	HDD	C3C-C4C-NC	-4.06	103.96	109.21
2	A	760	HDD	CAA-CBA-CGA	-4.04	105.34	112.75
2	B	760	HDD	C3C-C4C-NC	-4.02	104.01	109.21
2	A	760	HDD	C2D-C1D-CHD	-3.93	117.36	123.48
2	D	760	HDD	C3C-C4C-NC	-3.52	104.65	109.21
2	D	760	HDD	C3B-CAB-CBB	-3.47	119.21	126.32
2	C	760	HDD	C3C-C4C-NC	-2.96	105.38	109.21
2	C	760	HDD	O1D-CGD-CBD	-2.77	106.95	110.20
2	C	760	HDD	O1D-CGD-O2D	-2.46	118.46	120.80
2	D	760	HDD	CAA-C2A-C3A	-2.22	122.67	129.00
2	D	760	HDD	CMA-C3A-C4A	-2.09	124.91	128.36
2	C	760	HDD	CBA-CAA-C2A	2.29	116.63	112.53
2	A	760	HDD	CMA-C3A-C2A	2.31	130.07	125.24
2	C	760	HDD	CMA-C3A-C2A	2.61	130.70	125.24
2	D	760	HDD	C4D-ND-C1D	2.92	109.25	107.36
2	B	760	HDD	CMA-C3A-C2A	3.03	131.57	125.24
2	B	760	HDD	C4D-ND-C1D	3.18	109.41	107.36
2	C	760	HDD	C4D-ND-C1D	3.86	109.85	107.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HDD	7	0
2	B	760	HDD	5	0
2	C	760	HDD	5	0
2	D	760	HDD	4	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(Å^2)	Q<0.9
1	A	727/753 (96%)	-0.41	10 (1%)	78	80	2, 6, 21, 35	1 (0%)
1	B	727/753 (96%)	-0.35	14 (1%)	70	73	2, 7, 23, 33	1 (0%)
1	C	727/753 (96%)	-0.36	11 (1%)	76	79	2, 7, 23, 32	1 (0%)
1	D	727/753 (96%)	-0.44	8 (1%)	82	84	2, 7, 21, 33	1 (0%)
All	All	2908/3012 (96%)	-0.39	43 (1%)	76	79	2, 7, 22, 35	4 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	8.5
1	A	27	ASP	8.0
1	A	710	ILE	5.0
1	B	27	ASP	4.8
1	B	28	SER	4.8
1	C	28	SER	4.7
1	A	713	GLN	4.4
1	C	711	ALA	4.1
1	A	32	GLU	4.1
1	A	712	ASP	4.0
1	A	28	SER	3.9
1	D	27	ASP	3.6
1	D	750	LYS	3.6
1	D	28	SER	3.3
1	C	726	GLY	3.2
1	C	27	ASP	3.1
1	B	726	GLY	3.0
1	D	32	GLU	2.9
1	B	32	GLU	2.9
1	B	713	GLN	2.8
1	B	750	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	594	PRO	2.7
1	D	749	ASP	2.7
1	B	712	ASP	2.6
1	C	725	ASP	2.6
1	A	709	LYS	2.6
1	C	724	ALA	2.5
1	B	677	ASP	2.5
1	A	749	ASP	2.4
1	C	749	ASP	2.4
1	D	725	ASP	2.4
1	C	677	ASP	2.3
1	D	677	ASP	2.3
1	B	670	GLY	2.3
1	B	645	GLY	2.3
1	A	34	GLY	2.3
1	B	37	ARG	2.2
1	B	612	ARG	2.1
1	B	572	ASN	2.1
1	B	727	SER	2.1
1	C	750	LYS	2.1
1	D	751	ILE	2.0
1	C	703	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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(Å²)	Q<0.9
2	HDD	A	760	44/44	0.98	0.08	0.13	8,10,12,13	0
2	HDD	D	760	44/44	0.98	0.08	0.13	2,9,12,14	0
2	HDD	B	760	44/44	0.98	0.08	0.11	2,9,13,16	0
2	HDD	C	760	44/44	0.98	0.08	0.10	7,11,13,15	0

6.5 Other polymers (i)

There are no such residues in this entry.