Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:23 PM GMT

PDB ID	:	4ENQ
Title	:	Structure of E530D variant E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.90 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:

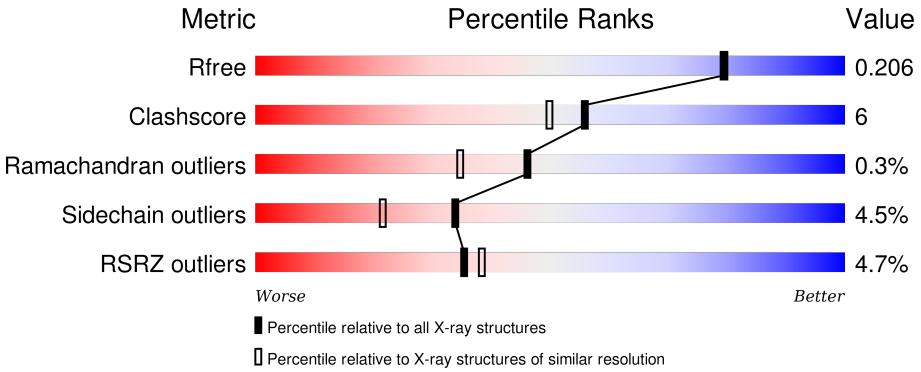
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	3% 85% 10%
1	B	753	9% 81% 12%
1	C	753	5% 79% 15%
1	D	753	2% 83% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26319 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.

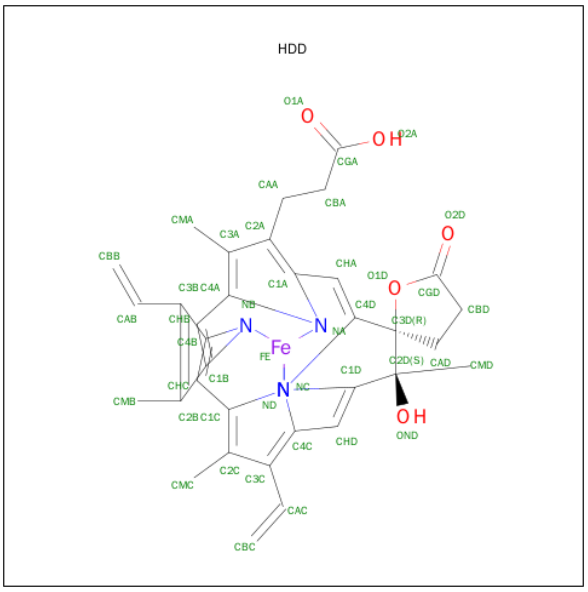
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	3	0
			5742	3643	1005	1082	12			
1	B	725	Total	C	N	O	S	0	3	0
			5746	3645	1006	1083	12			
1	C	725	Total	C	N	O	S	0	3	0
			5742	3643	1005	1082	12			
1	D	725	Total	C	N	O	S	0	3	0
			5746	3645	1006	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	ASP	GLU	ENGINEERED MUTATION	UNP P21179
B	530	ASP	GLU	ENGINEERED MUTATION	UNP P21179
C	530	ASP	GLU	ENGINEERED MUTATION	UNP P21179
D	530	ASP	GLU	ENGINEERED MUTATION	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.

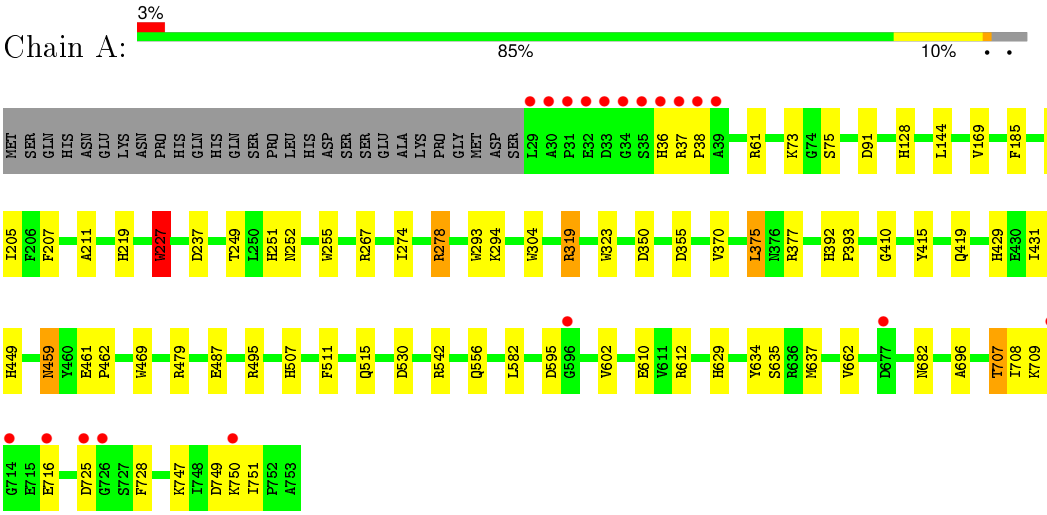
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	852	Total	O	0	0
			852	852		
3	B	705	Total	O	0	0
			705	705		
3	C	766	Total	O	0	0
			766	766		
3	D	844	Total	O	0	0
			844	844		

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.

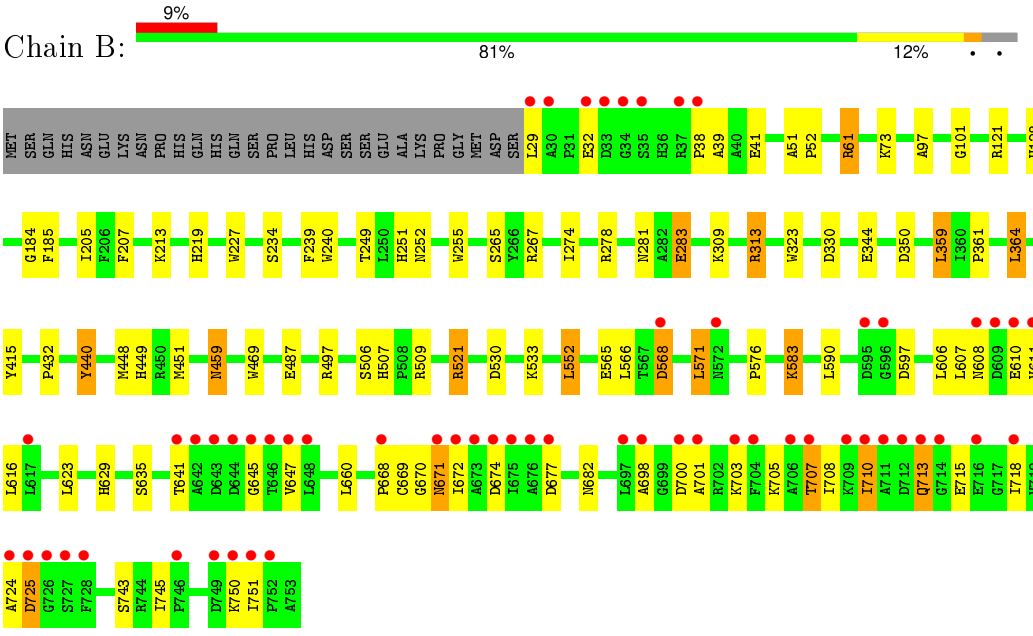
- Molecule 1: Catalase HPII

Chain A:



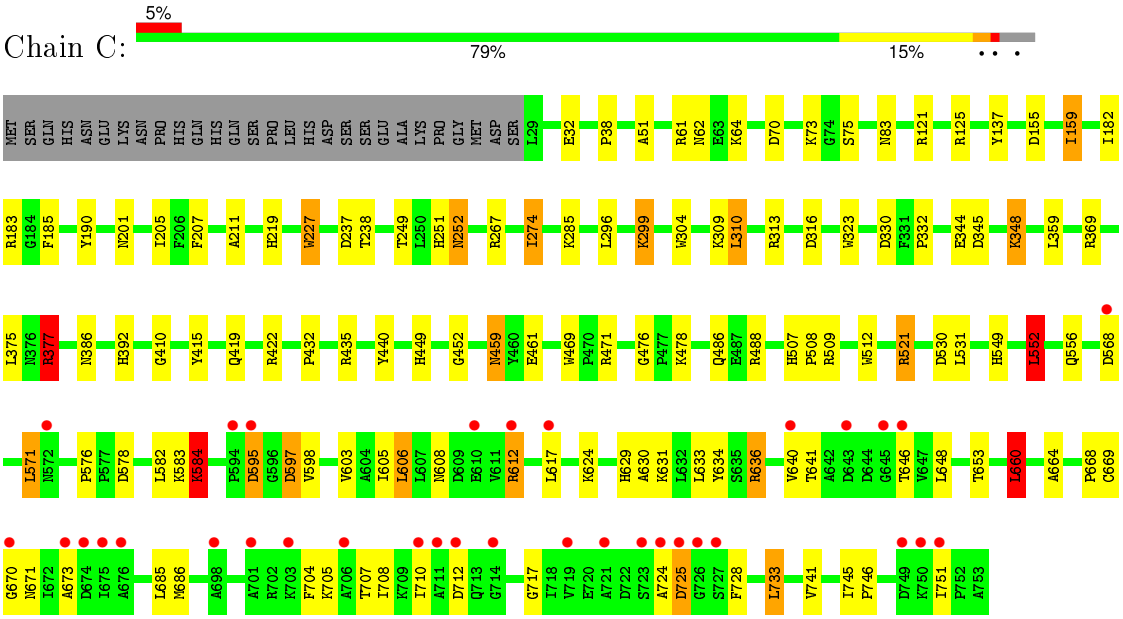
- Molecule 1: Catalase HPII

Chain B:



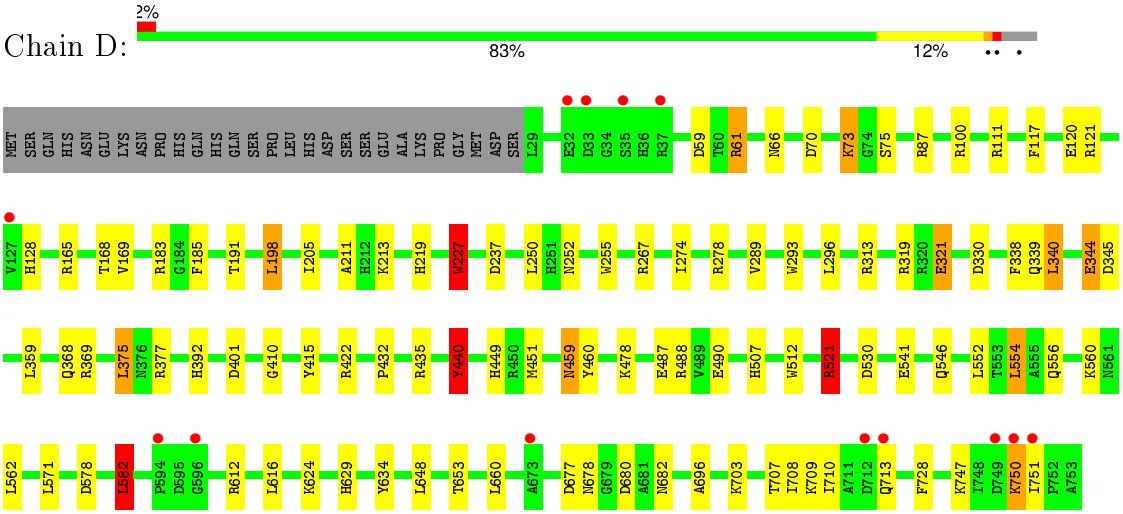
- Molecule 1: Catalase HPII

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	93.38Å 133.09Å 122.34Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	40.51 – 1.90 40.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (40.51-1.90) 92.1 (40.51-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.158 , 0.207 0.158 , 0.206	Depositor DCC
R_{free} test set	10217 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.1	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 204771 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26319	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, 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	1.06	7/5903 (0.1%)	0.96	13/8024 (0.2%)
1	B	1.00	5/5903 (0.1%)	0.94	8/8024 (0.1%)
1	C	1.01	6/5903 (0.1%)	0.97	15/8024 (0.2%)
1	D	1.03	5/5903 (0.1%)	1.00	20/8024 (0.2%)
All	All	1.03	23/23612 (0.1%)	0.97	56/32096 (0.2%)

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	440	TYR	CE1-CZ	8.03	1.49	1.38
1	A	440	TYR	CE1-CZ	7.27	1.48	1.38
1	D	293	TRP	CD2-CE2	6.32	1.49	1.41
1	B	469	TRP	CD2-CE2	6.15	1.48	1.41
1	C	304	TRP	CD2-CE2	5.84	1.48	1.41
1	B	323	TRP	CD2-CE2	5.78	1.48	1.41
1	B	440	TYR	CE1-CZ	5.64	1.45	1.38
1	C	512	TRP	CD2-CE2	5.54	1.48	1.41
1	D	512	TRP	CD2-CE2	5.50	1.48	1.41
1	D	227	TRP	CD2-CE2	5.49	1.48	1.41
1	C	344	GLU	CD-OE1	5.43	1.31	1.25
1	A	304	TRP	CD2-CE2	5.41	1.47	1.41
1	A	469	TRP	CD2-CE2	5.40	1.47	1.41
1	C	469	TRP	CD2-CE2	5.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	323	TRP	CD2-CE2	5.31	1.47	1.41
1	A	227	TRP	CD2-CE2	5.26	1.47	1.41
1	A	323	TRP	CD2-CE2	5.26	1.47	1.41
1	D	255	TRP	CD2-CE2	5.21	1.47	1.41
1	B	255	TRP	CD2-CE2	5.17	1.47	1.41
1	B	240	TRP	CD2-CE2	5.16	1.47	1.41
1	C	227	TRP	CD2-CE2	5.12	1.47	1.41
1	A	293	TRP	CD2-CE2	5.05	1.47	1.41
1	A	255	TRP	CD2-CE2	5.04	1.47	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ARG	NE-CZ-NH2	14.42	127.51	120.30
1	C	377	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	D	61	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	D	183	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	D	121	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	590	LEU	CB-CG-CD2	-6.99	99.12	111.00
1	D	377	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	D	198	LEU	CB-CG-CD1	6.76	122.49	111.00
1	C	435	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	D	521	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	479	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	313	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	C	70	ASP	CB-CG-OD2	6.48	124.14	118.30
1	A	294	LYS	CD-CE-NZ	-6.47	96.83	111.70
1	D	70	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	377	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	595	ASP	CB-CG-OD2	6.39	124.05	118.30
1	D	554	LEU	CB-CG-CD2	6.30	121.72	111.00
1	D	582	LEU	CB-CG-CD1	6.24	121.61	111.00
1	A	61	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	121	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	375	LEU	CB-CG-CD2	6.08	121.34	111.00
1	D	165	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	183	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	497	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	495	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	345	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	552	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	350	ASP	CB-CG-OD1	-5.83	113.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	155	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	595	ASP	CB-CG-OD2	5.75	123.48	118.30
1	D	87	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	401	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	348	LYS	CD-CE-NZ	-5.54	98.95	111.70
1	A	542	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	660	LEU	CB-CG-CD1	5.46	120.29	111.00
1	D	111	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	350	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	C	733	LEU	CA-CB-CG	5.38	127.66	115.30
1	A	355	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	D	344	GLU	CB-CA-C	-5.31	99.79	110.40
1	A	278	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	316	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	582	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	C	471	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	422	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	660	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	B	359	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	319	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	375	LEU	CB-CG-CD1	5.12	119.70	111.00
1	C	125	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	364	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	C	299	LYS	CD-CE-NZ	-5.10	99.98	111.70
1	C	121	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	121	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	422	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide

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	5742	0	5571	50	0
1	B	5746	0	5575	85	0
1	C	5742	0	5572	83	0
1	D	5746	0	5574	77	0
2	A	44	0	31	5	0
2	B	44	0	31	3	0
2	C	44	0	31	3	0
2	D	44	0	31	2	0
3	A	852	0	0	12	0
3	B	705	0	0	22	0
3	C	766	0	0	18	0
3	D	844	0	0	30	0
All	All	26319	0	22416	283	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 6.

All (283) 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:D:392:HIS:ND1	1:D:415:TYR:CB	1.70	1.50
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.71	1.50
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.77	1.47
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.77	1.45
1:B:449[A]:HIS:CE1	3:B:1602:HOH:O	1.70	1.28
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.69	1.27
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.24
1:B:449[A]:HIS:NE2	3:B:1602:HOH:O	1.58	1.22
1:D:546:GLN:HG3	3:D:1588:HOH:O	1.39	1.22
1:A:449[A]:HIS:CE1	3:A:1751:HOH:O	1.85	1.21
1:D:369:ARG:HD2	3:D:1742:HOH:O	1.35	1.20
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.78	1.19
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.84	1.16
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.16
3:B:1481:HOH:O	1:D:73:LYS:HD3	1.41	1.15
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.83	1.15
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.80	1.12
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.84	1.11
1:A:716:GLU:HG2	3:A:1685:HOH:O	1.54	1.05
1:D:709:LYS:HG3	1:D:750:LYS:HE3	1.38	1.04
1:C:267:ARG:HG3	3:C:1573:HOH:O	1.59	1.00
1:D:321:GLU:HG2	3:D:1424:HOH:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:HD2	3:C:1537:HOH:O	1.62	0.97
1:A:267:ARG:HG3	3:A:1730:HOH:O	1.66	0.94
1:D:321:GLU:CG	3:D:1424:HOH:O	2.17	0.89
1:A:612:ARG:HG3	3:A:1597:HOH:O	1.74	0.88
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.04	0.87
1:C:486:GLN:OE1	3:C:1570:HOH:O	1.94	0.86
1:B:61:ARG:HH11	1:B:61:ARG:CG	1.91	0.83
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.95	0.81
1:D:330:ASP:HA	3:D:1400:HOH:O	1.81	0.80
1:D:541:GLU:HG2	3:D:1684:HOH:O	1.83	0.78
1:B:73:LYS:HE3	1:D:440:TYR:O	1.85	0.77
1:B:583:LYS:NZ	1:B:583:LYS:H	1.81	0.77
1:B:61:ARG:HH11	1:B:61:ARG:HG3	1.49	0.76
1:D:267:ARG:HG3	3:D:1366:HOH:O	1.86	0.76
1:C:488:ARG:NH1	1:D:490:GLU:OE1	2.19	0.75
1:D:703:LYS:HE2	3:D:1589:HOH:O	1.85	0.74
1:D:629:HIS:HD2	3:D:1255:HOH:O	1.70	0.74
1:B:267:ARG:HG3	3:B:1370:HOH:O	1.88	0.73
1:A:278:ARG:HH12	1:A:487:GLU:CD	1.92	0.72
1:B:710:ILE:HD12	1:B:718:ILE:HG13	1.71	0.71
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.08	0.71
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.00	0.71
1:D:578:ASP:HB3	1:D:582:LEU:O	1.90	0.71
1:B:629:HIS:HD2	3:B:1166:HOH:O	1.73	0.70
1:B:724:ALA:O	1:B:725:ASP:O	2.10	0.69
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.75	0.69
1:A:556:GLN:NE2	3:A:1503:HOH:O	2.25	0.68
1:B:41:GLU:OE1	3:B:1485:HOH:O	2.10	0.68
1:B:73:LYS:CE	1:D:440:TYR:O	2.41	0.68
1:B:721:ALA:HB2	3:B:1258:HOH:O	1.93	0.68
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.25	0.67
1:D:61:ARG:NH1	3:D:1713:HOH:O	2.27	0.67
1:B:521:ARG:HH21	1:B:521:ARG:HG3	1.59	0.67
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.62	0.66
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.62	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.97	0.65
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.78	0.64
1:C:309:LYS:HE3	3:C:1175:HOH:O	1.98	0.63
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.28	0.63
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.01	0.63
1:C:478:LYS:HB2	3:C:1613:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.81	0.62
1:B:671:ASN:O	1:B:674:ASP:HB3	2.00	0.62
1:C:746:PRO:HG2	3:C:1521:HOH:O	2.00	0.61
1:C:578:ASP:HB2	1:C:582:LEU:O	2.02	0.60
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.49	0.60
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.43	0.59
1:C:313:ARG:HD2	3:C:1254:HOH:O	2.01	0.59
1:B:533:LYS:HE3	3:B:1259:HOH:O	2.02	0.58
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.85	0.58
1:B:583:LYS:HZ3	1:B:583:LYS:H	1.51	0.58
1:D:541:GLU:CG	3:D:1684:HOH:O	2.45	0.58
1:A:449[A]:HIS:NE2	3:A:1751:HOH:O	2.17	0.58
1:C:274:ILE:HD12	2:C:801:HDD:HMB1	1.86	0.57
1:D:521:ARG:HD3	3:D:1705:HOH:O	2.04	0.57
1:B:61:ARG:HG3	1:B:61:ARG:NH1	2.15	0.57
1:B:610:GLU:HB3	1:B:671:ASN:HB2	1.87	0.57
1:D:250:LEU:HD11	1:D:546:GLN:HE21	1.70	0.57
1:A:73:LYS:HE2	3:C:1142:HOH:O	2.04	0.56
1:C:629:HIS:HD2	3:C:1209:HOH:O	1.88	0.56
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.87	0.56
1:D:330:ASP:CA	3:D:1400:HOH:O	2.43	0.56
1:D:624:LYS:HD3	1:D:624:LYS:O	2.05	0.56
1:D:488:ARG:NE	3:D:1571:HOH:O	1.93	0.56
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.87	0.56
1:C:476:GLY:HA3	3:C:1281:HOH:O	2.04	0.56
1:B:610:GLU:HB3	1:B:671:ASN:CB	2.35	0.56
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.88	0.55
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.89	0.55
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.70	0.55
3:B:1481:HOH:O	1:D:73:LYS:CD	2.19	0.55
1:A:725:ASP:H	1:A:728:PHE:HB3	1.71	0.55
1:C:201:ASN:CG	2:C:801:HDD:HMB2	2.28	0.55
1:C:521:ARG:HG2	3:C:1575:HOH:O	2.06	0.54
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.88	0.54
1:C:636:ARG:NH1	3:C:1629:HOH:O	2.40	0.54
1:C:345:ASP:HA	1:C:348:LYS:HD2	1.89	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.22	0.54
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.68	0.54
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.90	0.53
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.53
1:D:556:GLN:NE2	3:D:1592:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.53
1:C:415:TYR:O	1:C:419:GLN:HG2	2.08	0.53
3:B:1338:HOH:O	1:D:449[A]:HIS:HE1	1.92	0.53
1:B:669:OCS:OD1	1:B:700:ASP:HB2	2.08	0.53
1:B:533:LYS:HE2	3:B:1550:HOH:O	2.09	0.52
1:B:29:LEU:N	3:B:1601:HOH:O	2.41	0.52
1:B:615:ASP:HA	1:B:724:ALA:HB3	1.90	0.52
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.75	0.52
1:C:313:ARG:HG3	1:C:660:LEU:HD23	1.92	0.52
1:A:751:ILE:O	1:A:751:ILE:HD12	2.08	0.52
1:C:267:ARG:HD3	1:C:332:PRO:HG3	1.92	0.51
1:B:612:ARG:O	1:B:615:ASP:HB2	2.11	0.51
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.91	0.51
1:B:698:ALA:H	1:B:701:ALA:HB3	1.74	0.51
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.10	0.51
1:C:73:LYS:CD	3:C:1537:HOH:O	2.39	0.51
1:D:267:ARG:CG	3:D:1366:HOH:O	2.52	0.51
1:C:32:GLU:HB2	3:C:1578:HOH:O	2.11	0.51
1:B:207:PHE:O	1:B:249:THR:HA	2.11	0.51
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.72	0.50
1:B:267:ARG:CG	3:B:1370:HOH:O	2.55	0.50
1:B:606:LEU:O	1:B:668:PRO:HD2	2.10	0.50
1:D:624:LYS:C	1:D:624:LYS:HD3	2.31	0.50
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.27	0.50
2:A:801:HDD:HBB1	2:A:801:HDD:HMB1	1.93	0.50
1:B:97:ALA:O	1:B:101:GLY:HA3	2.11	0.50
1:B:710:ILE:HG23	1:B:715:GLU:HB2	1.95	0.49
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.93	0.49
1:C:705:LYS:NZ	1:C:712:ASP:HA	2.27	0.49
1:D:368:GLN:HB3	3:D:1572:HOH:O	2.12	0.49
1:C:608:ASN:HA	1:C:634:TYR:HE1	1.77	0.49
1:B:29:LEU:HG	3:B:1601:HOH:O	2.13	0.48
1:C:62:ASN:C	1:C:62:ASN:OD1	2.51	0.48
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.48	0.48
1:C:251:HIS:HA	1:C:508:PRO:HG3	1.96	0.48
1:D:560:LYS:HD3	3:D:1717:HOH:O	2.14	0.48
1:B:52:PRO:HG3	3:D:1189:HOH:O	2.12	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.14	0.48
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.17	0.48
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.79	0.48
1:B:721:ALA:HB1	3:B:1555:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:CG	2:A:801:HDD:HMB2	2.34	0.48
1:B:713:GLN:CD	1:B:713:GLN:H	2.16	0.48
1:C:299:LYS:HE3	1:C:595:ASP:OD1	2.14	0.48
1:A:319:ARG:HD3	1:D:227:TRP:O	2.13	0.47
1:B:184:GLY:HA3	2:B:801:HDD:HMA2	1.96	0.47
1:A:511:PHE:O	1:A:515:GLN:HG2	2.14	0.47
1:C:745:ILE:HD13	3:C:1575:HOH:O	2.13	0.47
1:D:330:ASP:CB	3:D:1400:HOH:O	2.62	0.47
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.47
1:A:73:LYS:HD2	1:C:452:GLY:HA3	1.95	0.47
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.70	0.47
1:C:392:HIS:CG	1:C:415:TYR:CB	2.84	0.47
2:B:801:HDD:HBD2	3:B:1047:HOH:O	2.14	0.47
1:B:608:ASN:O	1:B:611:VAL:HG23	2.15	0.47
1:C:605:ILE:HD12	1:C:630:ALA:HB1	1.97	0.47
1:D:321:GLU:HG3	3:D:1424:HOH:O	2.03	0.47
2:C:801:HDD:HBD2	3:C:1088:HOH:O	2.14	0.47
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.47
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.97	0.46
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.50	0.46
1:B:309:LYS:CE	3:B:1132:HOH:O	2.64	0.46
1:C:669:OCS:SG	1:C:670:GLY:N	2.89	0.46
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.50	0.46
1:B:274:ILE:HD12	2:B:801:HDD:HMB1	1.97	0.46
1:D:359:LEU:H	1:D:507:HIS:HD2	1.63	0.46
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.46
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.46
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.98	0.46
1:D:488:ARG:NH2	3:D:1571:HOH:O	2.48	0.46
1:A:392:HIS:CE1	1:A:415:TYR:CB	2.68	0.46
1:B:448:MET:HG3	1:B:449[B]:HIS:CD2	2.50	0.46
1:C:64:LYS:HE2	1:C:190:TYR:CE1	2.51	0.46
1:A:716:GLU:CG	3:A:1685:HOH:O	2.34	0.45
2:A:801:HDD:HBD2	3:A:996:HOH:O	2.16	0.45
1:B:610:GLU:O	1:B:670:GLY:HA3	2.15	0.45
1:C:597:ASP:C	1:C:597:ASP:OD2	2.54	0.45
1:A:629:HIS:HE1	3:A:1495:HOH:O	1.98	0.45
1:B:521:ARG:HH21	1:B:521:ARG:CG	2.27	0.45
1:D:59:ASP:HB2	3:D:1318:HOH:O	2.15	0.45
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.52	0.45
1:C:207:PHE:CD2	1:C:252:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:LYS:HD3	1:D:751:ILE:HG12	1.97	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:B:392:HIS:ND1	1:B:415:TYR:CA	2.69	0.45
1:A:274:ILE:HD12	2:A:801:HDD:HMB1	1.98	0.45
1:B:359:LEU:H	1:B:507:HIS:HD2	1.65	0.45
1:A:207:PHE:O	1:A:249:THR:HA	2.17	0.44
1:C:597:ASP:OD2	1:C:598:VAL:N	2.50	0.44
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.53	0.44
1:B:506[B]:SER:OG	1:B:576:PRO:HB2	2.18	0.44
1:C:267:ARG:CD	1:C:332:PRO:HG3	2.47	0.44
1:A:392:HIS:CG	1:A:415:TYR:CB	2.83	0.44
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.44
1:D:435:ARG:HD3	3:D:1293:HOH:O	2.18	0.44
1:D:369:ARG:CD	3:D:1742:HOH:O	2.21	0.44
1:C:549:HIS:O	1:C:576:PRO:HD3	2.17	0.44
1:C:686:MET:CB	1:C:751:ILE:HD11	2.48	0.43
1:C:603:VAL:HG22	1:C:664:ALA:HB3	2.00	0.43
1:B:670:GLY:O	1:B:672:ILE:N	2.51	0.43
1:C:708:ILE:HG13	1:C:710:ILE:HG12	2.00	0.43
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.18	0.43
1:A:637:MET:HB2	1:D:562:LEU:HA	2.01	0.43
1:A:431:ILE:HG13	1:C:449[A]:HIS:CE1	2.53	0.43
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.43
1:B:647:VAL:O	1:B:647:VAL:HG12	2.18	0.43
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.43
1:A:602:VAL:HG13	1:A:662:VAL:HA	1.99	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.34	0.43
1:C:182:ILE:HG22	1:C:183:ARG:N	2.33	0.43
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.33	0.43
1:C:606:LEU:O	1:C:668:PRO:HD2	2.19	0.43
1:C:313:ARG:HG3	1:C:660:LEU:CD2	2.49	0.43
1:B:698:ALA:N	1:B:701:ALA:HB3	2.33	0.43
1:C:612:ARG:HD2	3:C:1610:HOH:O	2.17	0.43
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.00	0.43
1:A:278:ARG:HH21	1:A:278:ARG:HD2	1.70	0.43
1:D:117:PHE:HA	1:D:120:GLU:HG3	2.01	0.43
1:B:73:LYS:HE2	1:D:440:TYR:O	2.17	0.42
1:D:521:ARG:HG2	3:D:1629:HOH:O	2.19	0.42
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.02	0.42
1:D:296:LEU:HA	1:D:296:LEU:HD23	1.84	0.42
1:C:238:THR:HB	1:D:460:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ILE:HG13	1:B:700:ASP:CB	2.49	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.42
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.00	0.42
1:D:682:ASN:HB3	1:D:707:THR:HG21	2.01	0.42
2:D:801:HDD:HBD2	3:D:1139:HOH:O	2.19	0.42
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.50	0.42
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.36	0.42
2:A:801:HDD:HMC1	2:A:801:HDD:CBC	2.49	0.42
1:A:708:ILE:HG13	1:A:710:ILE:HG12	2.01	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:D:478:LYS:NZ	3:D:994:HOH:O	2.48	0.42
1:B:234:SER:HB2	1:B:239:PHE:CD2	2.54	0.42
1:B:671:ASN:ND2	1:B:674:ASP:HB2	2.34	0.42
1:A:36:HIS:HE1	3:A:1363:HOH:O	2.02	0.42
1:C:64:LYS:HE2	1:C:190:TYR:CZ	2.55	0.42
1:D:274:ILE:HD12	2:D:801:HDD:HMB1	2.02	0.42
1:B:267:ARG:NH1	3:B:1140:HOH:O	2.53	0.42
1:B:361:PRO:HD2	1:B:364:LEU:HD12	2.02	0.42
1:C:671:ASN:ND2	1:C:673:ALA:HB3	2.35	0.41
3:A:1172:HOH:O	1:D:100:ARG:HG3	2.18	0.41
1:A:634:TYR:CG	1:A:635:SER:N	2.88	0.41
1:A:37:ARG:HA	1:A:38:PRO:HD2	1.83	0.41
1:B:509:ARG:HD2	1:B:576:PRO:HD2	2.02	0.41
1:B:157:ASN:HB2	3:B:1554:HOH:O	2.19	0.41
1:D:578:ASP:HB2	3:D:1419:HOH:O	2.20	0.41
1:C:578:ASP:HB3	3:C:1574:HOH:O	2.20	0.41
1:C:717:GLY:HA3	1:C:741:VAL:HG11	2.02	0.41
1:B:330:ASP:OD1	1:B:629:HIS:HE1	2.03	0.41
1:B:713:GLN:NE2	1:B:713:GLN:H	2.18	0.41
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.03	0.41
1:C:686:MET:HB3	1:C:751:ILE:HD11	2.02	0.41
1:B:623:LEU:HD23	1:B:623:LEU:HA	1.73	0.41
1:D:678:ASN:OD1	1:D:680:ASP:HB2	2.21	0.41
1:D:128:HIS:HA	1:D:168:THR:O	2.20	0.41
1:D:521:ARG:CG	3:D:1629:HOH:O	2.68	0.41
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.56	0.41
1:A:610:GLU:HG3	3:A:1563:HOH:O	2.19	0.41
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.55	0.41
1:C:641:THR:HA	1:C:646:THR:O	2.21	0.41
1:B:451:MET:HE2	1:D:451:MET:HE1	2.02	0.41
1:B:743:SER:OG	3:B:1265:HOH:O	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1481:HOH:O	1:D:73:LYS:CG	2.64	0.40
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.74	0.40
1:B:313:ARG:HD2	3:B:1212:HOH:O	2.20	0.40
1:A:415:TYR:O	1:A:419:GLN:HG2	2.20	0.40
1:A:610:GLU:HA	1:A:610:GLU:OE1	2.21	0.40
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.03	0.40
1:D:289:VAL:HA	1:D:339:GLN:O	2.21	0.40
1:C:377:ARG:HD3	1:C:377:ARG:HH11	1.65	0.40
1:C:296:LEU:HA	1:C:296:LEU:HD23	1.90	0.40
1:C:509:ARG:HD3	1:C:576:PRO:HG2	2.02	0.40
1:A:227:TRP:O	1:D:319:ARG:HD3	2.22	0.40
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.64	0.40
1:C:634:TYR:O	1:C:653:THR:HA	2.21	0.40
1:B:641:THR:CG2	1:B:645:GLY:HA2	2.51	0.40
1:C:386:ASN:C	1:C:386:ASN:OD1	2.59	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%)	700 (97%)	24 (3%)	1 (0%)	56	46
1	B	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	30	17
1	C	725/753 (96%)	697 (96%)	24 (3%)	4 (1%)	30	17
1	D	725/753 (96%)	706 (97%)	18 (2%)	1 (0%)	56	46
All	All	2900/3012 (96%)	2803 (97%)	87 (3%)	10 (0%)	46	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	671	ASN
1	A	75	SER
1	B	705	LYS
1	C	75	SER
1	C	725	ASP
1	B	568	ASP
1	C	584	LYS
1	D	75	SER
1	C	274	ILE

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	612/635 (96%)	595 (97%)	17 (3%)	51	41
1	B	612/635 (96%)	581 (95%)	31 (5%)	29	17
1	C	612/635 (96%)	577 (94%)	35 (6%)	25	13
1	D	612/635 (96%)	585 (96%)	27 (4%)	35	22
All	All	2448/2540 (96%)	2338 (96%)	110 (4%)	34	21

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	530	ASP
1	A	707	THR

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Mol	Chain	Res	Type
1	A	709	LYS
1	A	713	GLN
1	A	747	LYS
1	A	749	ASP
1	A	750	LYS
1	B	61	ARG
1	B	185	PHE
1	B	205	ILE
1	B	213	LYS
1	B	227	TRP
1	B	252	ASN
1	B	265	SER
1	B	283	GLU
1	B	344	GLU
1	B	375	LEU
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	530	ASP
1	B	552	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	597	ASP
1	B	612	ARG
1	B	635	SER
1	B	677	ASP
1	B	703	LYS
1	B	707	THR
1	B	710	ILE
1	B	713	GLN
1	B	750	LYS
1	B	751	ILE
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP

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Mol	Chain	Res	Type
1	C	252	ASN
1	C	285	LYS
1	C	310	LEU
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	521	ARG
1	C	530	ASP
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	597	ASP
1	C	606	LEU
1	C	612	ARG
1	C	617	LEU
1	C	624	LYS
1	C	631	LYS
1	C	633	LEU
1	C	636	ARG
1	C	640	VAL
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	733	LEU
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	213	LYS
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	321	GLU
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU

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Mol	Chain	Res	Type
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	521	ARG
1	D	530	ASP
1	D	554	LEU
1	D	582	LEU
1	D	612	ARG
1	D	616	LEU
1	D	648	LEU
1	D	677	ASP
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	556	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	486	GLN
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	459	ASN
1	D	507	HIS
1	D	556	GLN

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Mol	Chain	Res	Type
1	D	629	HIS
1	D	671	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	A	669	1	7,8,9	3.90	2 (28%)	7,11,13	3.72	4 (57%)
1	OCS	B	669	1	7,8,9	3.52	2 (28%)	7,11,13	4.37	2 (28%)
1	OCS	C	669	1	7,8,9	3.41	2 (28%)	7,11,13	1.76	1 (14%)
1	OCS	D	669	1	7,8,9	2.89	2 (28%)	7,11,13	2.98	2 (28%)

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
1	OCS	A	669	1	-	1/4/7/9	0/0/0/0
1	OCS	B	669	1	-	1/4/7/9	0/0/0/0
1	OCS	C	669	1	-	1/4/7/9	0/0/0/0
1	OCS	D	669	1	-	1/4/7/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	OCS	CB-SG	-7.95	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	CB-SG	-6.30	1.68	1.77
1	C	669	OCS	CB-SG	-5.72	1.69	1.77
1	D	669	OCS	CB-SG	-4.74	1.70	1.77
1	D	669	OCS	OD2-SG	5.88	1.61	1.46
1	A	669	OCS	OD2-SG	6.41	1.63	1.46
1	B	669	OCS	OD2-SG	6.66	1.63	1.46
1	C	669	OCS	OD2-SG	6.76	1.63	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	669	OCS	OD3-SG-CB	-4.27	103.34	106.94
1	A	669	OCS	OD2-SG-OD3	-4.14	101.98	111.61
1	B	669	OCS	OD3-SG-CB	-3.42	104.06	106.94
1	A	669	OCS	OD3-SG-CB	-2.95	104.46	106.94
1	A	669	OCS	CB-CA-C	2.42	118.08	111.46
1	C	669	OCS	OD3-SG-CB	3.01	109.48	106.94
1	D	669	OCS	OD1-SG-CB	6.14	112.12	106.94
1	A	669	OCS	OD1-SG-CB	7.86	113.56	106.94
1	B	669	OCS	OD1-SG-CB	10.61	115.89	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	669	OCS	SG-CB-CA-N
1	C	669	OCS	SG-CB-CA-N
1	A	669	OCS	SG-CB-CA-N
1	D	669	OCS	SG-CB-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0
1	C	669	OCS	1	0

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	801	1,3	30,52,52	2.14	8 (26%)	20,89,89	3.54	6 (30%)
2	HDD	B	801	1,3	30,52,52	2.31	8 (26%)	20,89,89	3.76	10 (50%)
2	HDD	C	801	1,3	30,52,52	2.33	9 (30%)	20,89,89	3.42	11 (55%)
2	HDD	D	801	1	30,52,52	2.33	10 (33%)	20,89,89	3.50	12 (60%)

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	801	1,3	-	0/3/89/89	0/1/9/9
2	HDD	B	801	1,3	-	0/3/89/89	0/1/9/9
2	HDD	C	801	1,3	-	0/3/89/89	0/1/9/9
2	HDD	D	801	1	-	0/3/89/89	0/1/9/9

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HDD	C4B-NB	-2.46	1.33	1.36
2	D	801	HDD	C4B-NB	-2.25	1.33	1.36
2	D	801	HDD	C2A-C3A	2.02	1.43	1.37
2	D	801	HDD	C1C-CHC	2.04	1.45	1.39
2	A	801	HDD	CMC-C2C	2.13	1.56	1.51
2	D	801	HDD	OND-C2D	2.14	1.47	1.42
2	D	801	HDD	C4A-CHB	2.29	1.46	1.39
2	B	801	HDD	C1A-CHA	2.31	1.46	1.39
2	C	801	HDD	C1C-CHC	2.59	1.47	1.39
2	C	801	HDD	C4C-CHD	2.71	1.47	1.39
2	B	801	HDD	C4A-CHB	2.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HDD	C2A-C3A	2.76	1.45	1.37
2	A	801	HDD	C3C-C2C	2.84	1.44	1.40
2	A	801	HDD	C4C-CHD	2.86	1.47	1.39
2	C	801	HDD	C4A-CHB	2.97	1.48	1.39
2	D	801	HDD	C4C-CHD	3.06	1.48	1.39
2	C	801	HDD	C2A-C3A	3.21	1.47	1.37
2	B	801	HDD	C4C-CHD	3.22	1.48	1.39
2	A	801	HDD	C1C-CHC	3.23	1.48	1.39
2	C	801	HDD	O1D-C3D	3.27	1.52	1.46
2	D	801	HDD	C3C-C2C	3.39	1.44	1.40
2	A	801	HDD	C1A-CHA	3.40	1.49	1.39
2	C	801	HDD	C1A-CHA	3.60	1.49	1.39
2	C	801	HDD	O1D-CGD	4.00	1.42	1.35
2	A	801	HDD	C3B-C2B	4.03	1.45	1.40
2	C	801	HDD	C3B-C2B	4.20	1.45	1.40
2	B	801	HDD	O1D-CGD	4.37	1.43	1.35
2	D	801	HDD	O1D-C3D	4.46	1.54	1.46
2	B	801	HDD	C3C-C2C	4.74	1.46	1.40
2	B	801	HDD	O1D-C3D	5.47	1.56	1.46
2	B	801	HDD	C3B-C2B	6.12	1.48	1.40
2	D	801	HDD	O1D-CGD	6.15	1.46	1.35
2	A	801	HDD	O1D-CGD	6.42	1.46	1.35
2	D	801	HDD	C3B-C2B	6.74	1.49	1.40
2	C	801	HDD	C3C-C2C	7.39	1.50	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HDD	C3C-CAC-CBC	-7.78	110.40	126.32
2	C	801	HDD	C4D-ND-C1D	-6.50	103.17	107.36
2	B	801	HDD	CAA-CBA-CGA	-6.03	101.69	112.75
2	D	801	HDD	C3C-CAC-CBC	-5.99	114.07	126.32
2	C	801	HDD	C3B-CAB-CBB	-5.92	114.20	126.32
2	D	801	HDD	OND-C2D-CMD	-5.92	98.73	109.41
2	C	801	HDD	OND-C2D-CMD	-5.88	98.80	109.41
2	D	801	HDD	C4D-ND-C1D	-5.71	103.68	107.36
2	A	801	HDD	OND-C2D-CMD	-5.66	99.19	109.41
2	B	801	HDD	OND-C2D-CMD	-5.22	99.98	109.41
2	A	801	HDD	O1D-CGD-CBD	-5.13	104.19	110.20
2	C	801	HDD	CAA-CBA-CGA	-5.05	103.49	112.75
2	D	801	HDD	CAA-CBA-CGA	-4.86	103.84	112.75
2	A	801	HDD	CAA-CBA-CGA	-4.38	104.71	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HDD	C4D-ND-C1D	-4.31	104.58	107.36
2	C	801	HDD	O1D-CGD-CBD	-4.23	105.25	110.20
2	A	801	HDD	C4D-ND-C1D	-4.23	104.63	107.36
2	D	801	HDD	C3B-CAB-CBB	-4.03	118.07	126.32
2	D	801	HDD	C2D-C1D-CHD	-3.48	118.05	123.48
2	B	801	HDD	O1D-CGD-CBD	-3.34	106.29	110.20
2	B	801	HDD	CBA-CAA-C2A	-3.20	106.79	112.53
2	C	801	HDD	CBA-CAA-C2A	-3.18	106.83	112.53
2	D	801	HDD	O1D-CGD-CBD	-3.04	106.64	110.20
2	B	801	HDD	C2D-C1D-CHD	-2.87	119.01	123.48
2	C	801	HDD	C3C-CAC-CBC	-2.66	120.89	126.32
2	B	801	HDD	C3C-CAC-CBC	-2.31	121.59	126.32
2	D	801	HDD	CBA-CAA-C2A	-2.30	108.40	112.53
2	D	801	HDD	C3C-C4C-NC	2.04	111.85	109.21
2	C	801	HDD	CMC-C2C-C1C	2.08	131.81	128.36
2	D	801	HDD	CMB-C2B-C3B	2.17	129.33	125.09
2	B	801	HDD	CMA-C3A-C2A	2.21	129.86	125.24
2	C	801	HDD	CMB-C2B-C3B	2.32	129.63	125.09
2	D	801	HDD	CMC-C2C-C1C	2.38	132.30	128.36
2	C	801	HDD	CMA-C3A-C2A	2.92	131.34	125.24
2	B	801	HDD	CMC-C2C-C3C	3.81	132.54	125.09
2	C	801	HDD	O1D-CGD-O2D	6.05	126.55	120.80
2	D	801	HDD	O1D-CGD-O2D	7.32	127.76	120.80
2	A	801	HDD	O1D-CGD-O2D	8.77	129.15	120.80
2	B	801	HDD	O1D-CGD-O2D	11.35	131.60	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HDD	5	0
2	B	801	HDD	3	0
2	C	801	HDD	3	0
2	D	801	HDD	2	0

5.7 Other polymers (i)

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	724/753 (96%)	-0.37	22 (3%)	54	57	4, 10, 31, 76	1 (0%)
1	B	724/753 (96%)	0.08	66 (9%)	11	13	5, 13, 58, 76	1 (0%)
1	C	724/753 (96%)	-0.12	34 (4%)	35	38	5, 12, 46, 70	1 (0%)
1	D	724/753 (96%)	-0.26	13 (1%)	71	74	4, 11, 28, 64	0
All	All	2896/3012 (96%)	-0.17	135 (4%)	35	38	4, 11, 45, 76	3 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	8.3
1	A	32	GLU	6.0
1	B	750	LYS	5.9
1	B	32	GLU	4.9
1	B	677	ASP	4.9
1	B	672	ILE	4.8
1	B	714	GLY	4.7
1	A	710	ILE	4.6
1	C	675	ILE	4.6
1	B	34	GLY	4.6
1	C	711	ALA	4.5
1	A	35	SER	4.5
1	B	711	ALA	4.4
1	C	701	ALA	4.2
1	B	712	ASP	4.1
1	A	36	HIS	4.1
1	B	751	ILE	4.1
1	C	726	GLY	4.0
1	D	750	LYS	4.0
1	B	701	ALA	3.9
1	A	33	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	721	ALA	3.8
1	A	39	ALA	3.8
1	B	713	GLN	3.8
1	B	675	ILE	3.8
1	A	714	GLY	3.7
1	C	724	ALA	3.6
1	C	721	ALA	3.6
1	B	30	ALA	3.6
1	C	698	ALA	3.5
1	B	722	ASP	3.5
1	B	646	THR	3.5
1	A	37	ARG	3.5
1	B	698	ALA	3.5
1	A	29	LEU	3.4
1	B	29	LEU	3.4
1	A	34	GLY	3.4
1	B	608	ASN	3.3
1	B	614	ALA	3.3
1	B	725	ASP	3.3
1	C	750	LYS	3.2
1	C	727	SER	3.2
1	C	751	ILE	3.2
1	B	611	VAL	3.2
1	B	33	ASP	3.1
1	B	37	ARG	3.1
1	C	706	ALA	3.1
1	B	727	SER	3.1
1	B	700	ASP	3.1
1	B	720	GLU	3.0
1	D	32	GLU	3.0
1	B	647	VAL	3.0
1	B	572	ASN	3.0
1	B	704	PHE	2.9
1	B	728	PHE	2.9
1	C	594	PRO	2.9
1	C	676	ALA	2.9
1	B	749	ASP	2.9
1	B	612	ARG	2.9
1	A	38	PRO	2.9
1	B	723	SER	2.9
1	B	643	ASP	2.9
1	B	609	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	725	ASP	2.8
1	A	30	ALA	2.8
1	C	712	ASP	2.8
1	C	714	GLY	2.7
1	A	31	PRO	2.7
1	B	35	SER	2.7
1	B	673	ALA	2.7
1	C	612	ARG	2.7
1	B	645	GLY	2.7
1	D	713	GLN	2.7
1	D	35	SER	2.6
1	B	644	ASP	2.6
1	C	568	ASP	2.6
1	A	713	GLN	2.6
1	B	671	ASN	2.6
1	B	709	LYS	2.6
1	B	676	ALA	2.5
1	C	617	LEU	2.5
1	D	749	ASP	2.5
1	D	751	ILE	2.5
1	C	719	VAL	2.5
1	C	610	GLU	2.5
1	B	38	PRO	2.5
1	B	668	PRO	2.5
1	A	711	ALA	2.4
1	C	572	ASN	2.4
1	B	707	THR	2.4
1	B	617	LEU	2.4
1	C	673	ALA	2.4
1	B	706	ALA	2.3
1	A	726	GLY	2.3
1	D	594	PRO	2.3
1	A	712	ASP	2.3
1	B	610	GLU	2.3
1	B	746	PRO	2.3
1	C	646	THR	2.3
1	A	596	GLY	2.3
1	B	615	ASP	2.3
1	B	674	ASP	2.2
1	D	37	ARG	2.2
1	C	595	ASP	2.2
1	D	712	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	697	LEU	2.2
1	C	749	ASP	2.2
1	D	127	VAL	2.2
1	B	641	THR	2.2
1	C	640	VAL	2.2
1	C	723	SER	2.2
1	D	596	GLY	2.2
1	B	568	ASP	2.1
1	B	710	ILE	2.1
1	B	718	ILE	2.1
1	A	725	ASP	2.1
1	C	670	GLY	2.1
1	B	703	LYS	2.1
1	B	724	ALA	2.1
1	D	673	ALA	2.1
1	A	677	ASP	2.1
1	B	595	ASP	2.1
1	C	674	ASP	2.1
1	D	33	ASP	2.1
1	B	648	LEU	2.1
1	C	645	GLY	2.1
1	C	710	ILE	2.0
1	B	596	GLY	2.0
1	A	716	GLU	2.0
1	A	750	LYS	2.0
1	B	716	GLU	2.0
1	C	703	LYS	2.0
1	B	642	ALA	2.0
1	C	643	ASP	2.0
1	B	752	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	OCS	C	669	9/10	0.84	0.30	-	54,59,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	OCS	D	669	9/10	0.95	0.15	-	22,24,32,38	0
1	OCS	A	669	9/10	0.92	0.14	-	18,21,35,36	0
1	OCS	B	669	9/10	0.78	0.34	-	56,66,70,72	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HDD	B	801	44/44	0.96	0.10	0.51	7,9,14,17	0
2	HDD	C	801	44/44	0.97	0.10	0.12	6,10,14,16	0
2	HDD	D	801	44/44	0.97	0.12	0.12	5,7,10,12	0
2	HDD	A	801	44/44	0.97	0.09	-0.10	5,8,12,16	0

6.5 Other polymers (i)

There are no such residues in this entry.