Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:00 PM EDT

PDB ID	:	4V3F
Title	:	Crystal structure of betaine aldehyde dehydrogenase from spinach showing a thiohemiacetal with betaine aldehyde
Authors	:	Zarate-Romero, A.; Munoz-Clares, R.A.
Deposited on	:	2014-10-18
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

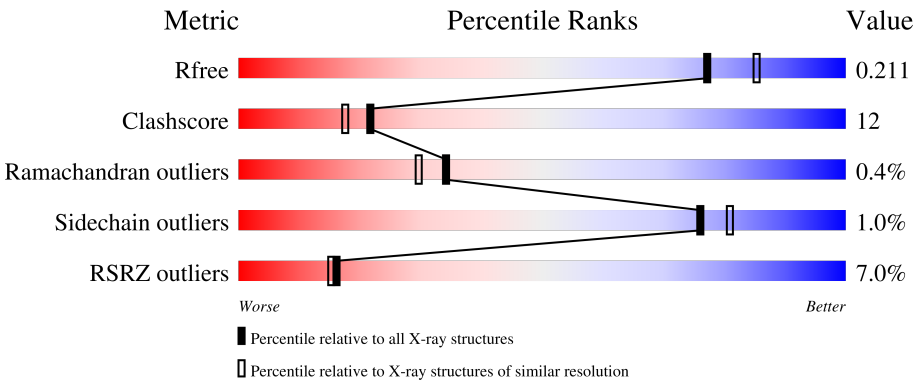
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	498	5% 79% 20% •
1	B	498	7% 75% 23% ••
1	D	498	6% 82% 17% •
2	C	497	9% 75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	B	1498	-	-	X	-
3	IOD	C	1499	-	-	X	-
4	CHT	A	1502	-	-	X	-
4	CHT	D	1501	-	-	X	-
5	PG4	D	1502	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16235 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 BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	3861	2475	641	726	19	0	7	0
1	B	494	3899	2494	658	728	19	0	11	0
1	D	495	3853	2472	640	723	18	0	7	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	CSO	CYS	microheterogeneity	UNP P17202
B	291	CSO	CYS	microheterogeneity	UNP P17202
D	291	CSO	CYS	microheterogeneity	UNP P17202

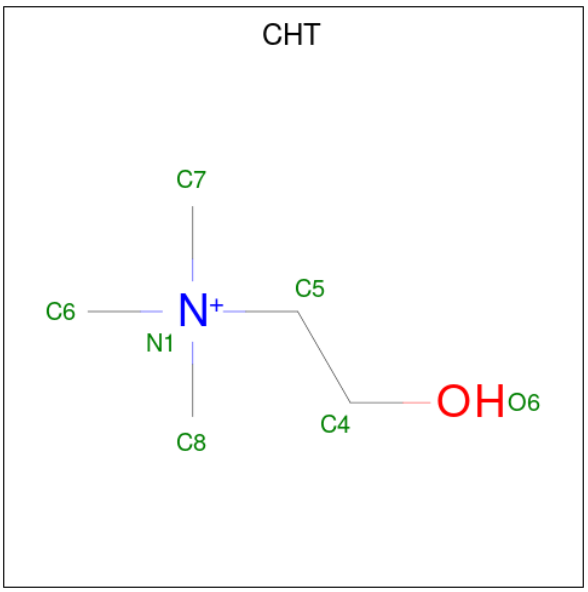
- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	495	3871	2478	647	729	17	0	7	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

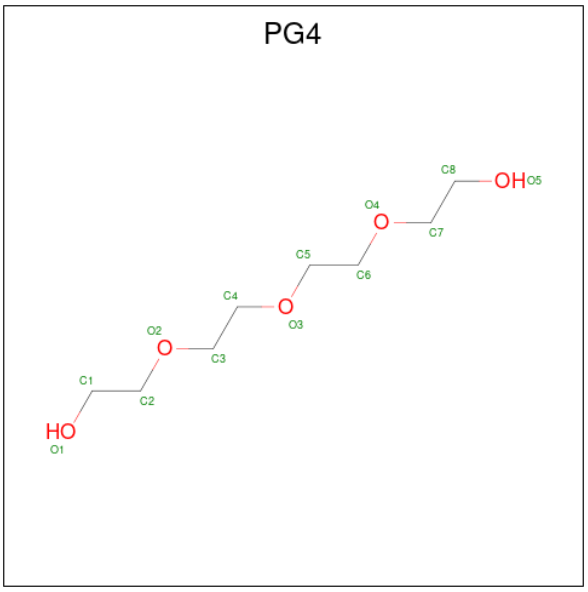
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
3	A	5	5	5	0	0
3	B	4	4	4	0	0
3	C	3	3	3	0	0
3	D	3	3	3	0	0

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).



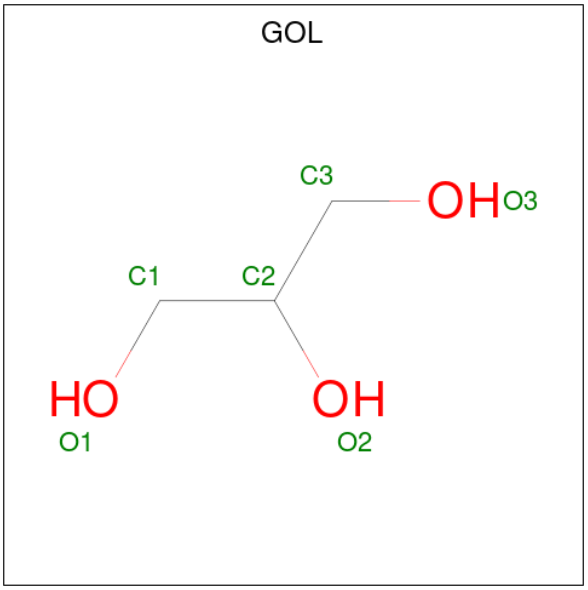
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	7	5	1	1	0	0
4	B	1	7	5	1	1	0	0
4	D	1	7	5	1	1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



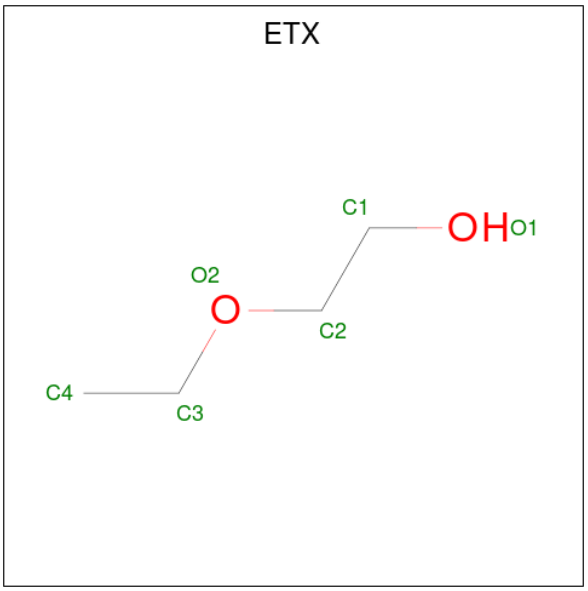
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			12	8	4			
5	C	1	Total	C	O		0	0
			12	8	4			
5	D	1	Total	C	O		0	0
			12	8	4			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O		0	0
			6	3	3			
6	D	1	Total	C	O		0	0
			6	3	3			

- Molecule 7 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	6	4	2	0	0

- Molecule 8 is water.

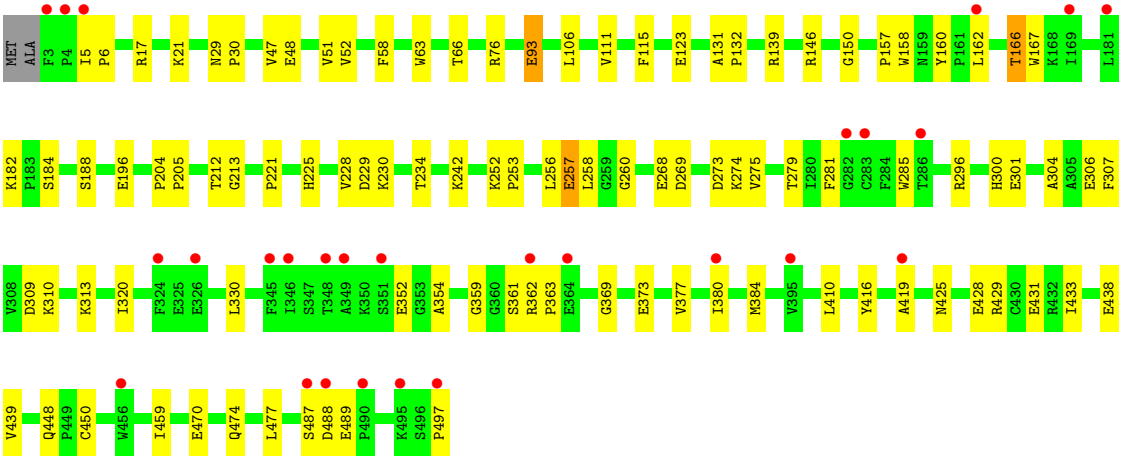
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	189	189	189	0	0
			Total	O		
8	B	130	130	130	0	0
			Total	O		
8	C	163	163	163	0	0
			Total	O		
8	D	179	179	179	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

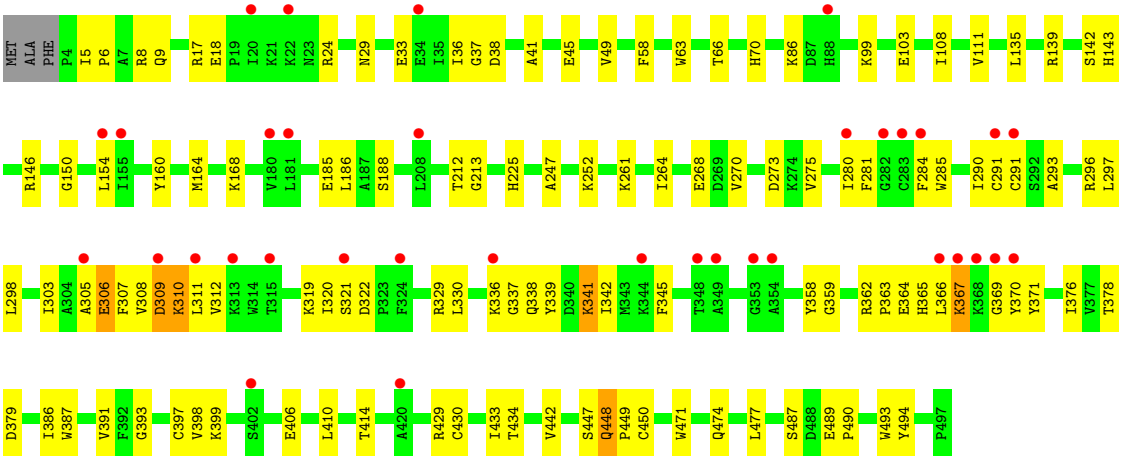
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain A:



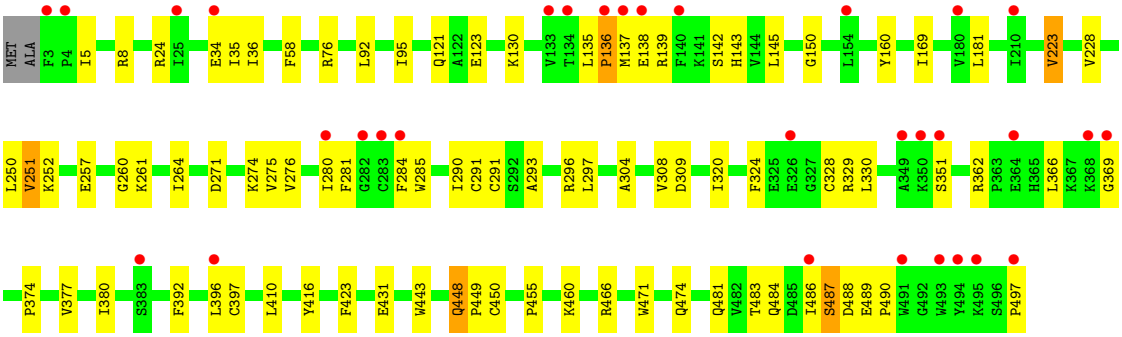
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain B:



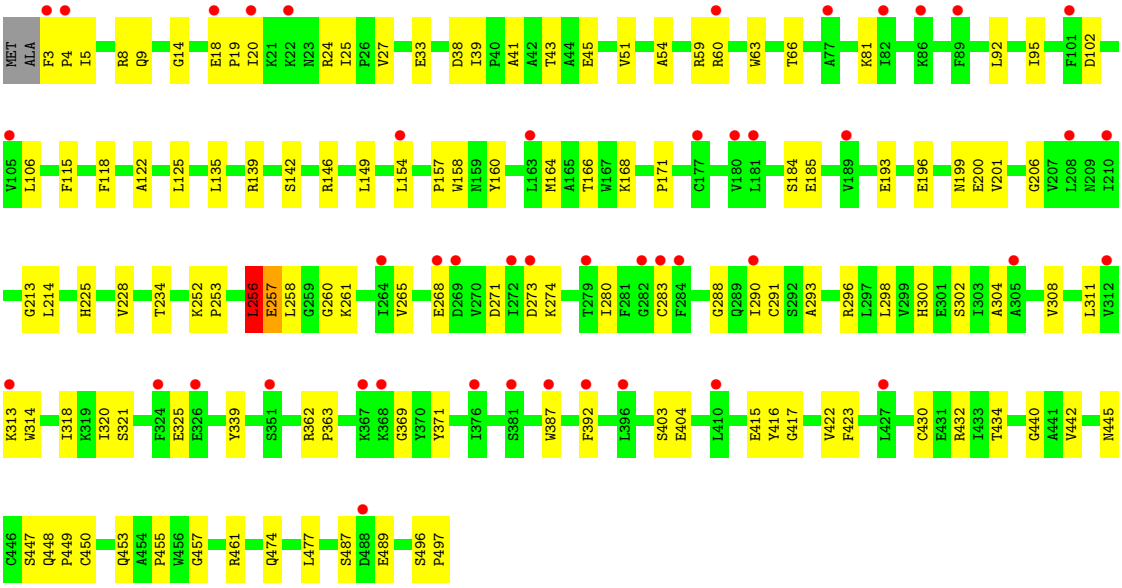
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain D:



- Molecule 2: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.44Å 82.26Å 88.52Å 79.44° 84.89° 77.32°	Depositor
Resolution (Å)	28.97 – 2.00 29.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.97-2.00) 96.1 (29.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.196 , 0.211 0.198 , 0.211	Depositor DCC
R_{free} test set	5969 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16235	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.333 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: ETX, CSO, IOD, PG4, CHT, GOL

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	0.47	0/3946	0.60	1/5366 (0.0%)
1	B	0.43	0/3983	0.59	0/5412
1	D	0.47	0/3939	0.61	2/5359 (0.0%)
2	C	0.41	0/3946	0.61	3/5364 (0.1%)
All	All	0.45	0/15814	0.60	6/21501 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	C	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	256	LEU	O-C-N	-11.12	104.90	122.70
2	C	497	PRO	N-CA-CB	7.41	112.19	103.30
2	C	256	LEU	CA-C-N	7.00	132.61	117.20
1	A	497	PRO	N-CA-CB	5.93	110.42	103.30
1	D	497	PRO	N-CA-CB	5.83	110.30	103.30
1	D	250	LEU	O-C-N	-5.22	114.34	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166[B]	THR	Mainchain
2	C	256	LEU	Mainchain
1	D	396	LEU	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	3861	0	3839	81	0
1	B	3899	0	3899	121	0
1	D	3853	0	3848	66	0
2	C	3871	0	3856	97	0
3	A	5	0	0	2	0
3	B	4	0	0	4	0
3	C	3	0	0	4	0
3	D	3	0	0	1	0
4	A	7	0	12	9	0
4	B	7	0	12	5	0
4	D	7	0	12	6	0
5	A	12	0	15	0	0
5	C	12	0	15	0	0
5	D	12	0	15	10	0
6	B	6	0	8	0	0
6	D	6	0	8	3	0
7	C	6	0	10	0	0
8	A	189	0	0	9	0
8	B	130	0	0	6	0
8	C	163	0	0	7	0
8	D	179	0	0	2	0
All	All	16235	0	15549	367	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 12.

All (367) 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:336:LYS:HD2	1:B:370:TYR:CE1	1.17	1.63
1:B:336:LYS:CD	1:B:370:TYR:HE1	1.10	1.55
1:B:336:LYS:CD	1:B:370:TYR:CE1	1.80	1.49
1:A:450[B]:CYS:HB2	4:A:1502:CHT:C4	1.59	1.32
2:C:81:LYS:NZ	2:C:200:GLU:HB3	1.49	1.27
1:A:487:SER:O	1:A:488:ASP:OD1	1.54	1.23
1:B:450[B]:CYS:HB2	4:B:1501:CHT:C4	1.78	1.14
1:B:337:GLY:O	1:B:341:LYS:HE2	1.56	1.06
2:C:321:SER:HB2	2:C:325:GLU:OE1	1.55	1.05
1:B:336:LYS:CD	1:B:370:TYR:CZ	2.38	1.05
1:B:336:LYS:HD3	1:B:370:TYR:CE1	1.92	1.01
1:B:336:LYS:CG	1:B:370:TYR:CE1	2.46	0.98
1:B:336:LYS:HG2	1:B:370:TYR:CZ	2.00	0.96
1:D:121:GLN:NE2	8:D:2071:HOH:O	2.00	0.95
1:A:450[B]:CYS:HB2	4:A:1502:CHT:HC41	0.94	0.94
2:C:81:LYS:HZ2	2:C:200:GLU:HB3	1.32	0.94
2:C:81:LYS:HZ3	2:C:200:GLU:HB3	1.15	0.92
2:C:81:LYS:NZ	2:C:200:GLU:CB	2.33	0.92
1:A:115:PHE:CE2	1:A:166[B]:THR:HG23	2.04	0.91
1:B:336:LYS:HD3	1:B:370:TYR:CZ	2.05	0.90
1:B:146[B]:ARG:NH1	8:B:2063:HOH:O	2.05	0.89
1:B:336:LYS:HD3	1:B:370:TYR:OH	1.70	0.89
1:B:362:ARG:NH2	1:B:369:GLY:O	2.06	0.89
1:B:303:ILE:C	1:B:306:GLU:OE1	2.11	0.88
1:B:336:LYS:CG	1:B:370:TYR:CZ	2.59	0.86
2:C:81:LYS:HZ2	2:C:200:GLU:CB	1.89	0.85
2:C:474:GLN:NE2	3:C:1499:IOD:I	2.80	0.85
1:B:261:LYS:O	1:B:296:ARG:NH1	2.09	0.84
2:C:81:LYS:NZ	2:C:200:GLU:C	2.30	0.84
2:C:158:TRP:CZ2	2:C:392:PHE:HE2	1.97	0.83
2:C:257[A]:GLU:OE2	2:C:291:CSO:OD	1.96	0.83
1:A:111:VAL:HG13	1:A:166[A]:THR:HG21	1.62	0.82
2:C:24:ARG:NE	2:C:38:ASP:OD2	2.11	0.82
2:C:81:LYS:NZ	2:C:200:GLU:O	2.13	0.81
1:D:8:ARG:O	1:D:24:ARG:NH2	2.11	0.81
1:A:487:SER:O	1:A:488:ASP:CG	2.19	0.81
2:C:403:SER:OG	8:C:2134:HOH:O	2.00	0.78
1:D:138:GLU:OE2	8:D:2076:HOH:O	2.01	0.78
1:B:337:GLY:O	1:B:341:LYS:CE	2.32	0.77
1:A:242:LYS:NZ	8:A:2115:HOH:O	2.15	0.76
1:A:196:GLU:OE2	8:A:2010:HOH:O	2.02	0.76
2:C:268:GLU:OE2	2:C:300:HIS:CE1	2.39	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:NH2	1:A:410:LEU:O	2.18	0.76
2:C:362:ARG:NH2	2:C:369:GLY:O	2.18	0.76
2:C:102:ASP:O	2:C:106:LEU:HD12	1.86	0.74
1:B:336:LYS:HD2	1:B:370:TYR:CD1	2.14	0.73
1:A:139:ARG:NH2	1:A:489:GLU:O	2.22	0.73
2:C:81:LYS:HZ2	2:C:200:GLU:C	1.92	0.72
1:D:466:ARG:HG2	5:D:1502:PG4:H71	1.71	0.71
1:B:434:THR:HG22	1:B:442:VAL:HG11	1.73	0.71
2:C:268:GLU:CD	2:C:302:SER:OG	2.29	0.71
1:B:378:THR:HG22	1:B:379:ASP:H	1.56	0.70
1:A:474:GLN:HG3	8:A:2181:HOH:O	1.91	0.70
2:C:185:GLU:HG3	2:C:214:LEU:HD23	1.74	0.69
2:C:268:GLU:OE1	2:C:302:SER:OG	2.10	0.69
1:B:336:LYS:CD	1:B:370:TYR:OH	2.38	0.68
2:C:18:GLU:HG2	2:C:19:PRO:HD2	1.74	0.68
1:A:115:PHE:CE2	1:A:166[B]:THR:CG2	2.77	0.68
1:D:449:PRO:HA	6:D:1503:GOL:H31	1.73	0.68
1:B:261:LYS:HG3	1:B:296:ARG:HH11	1.59	0.68
2:C:158:TRP:CZ2	2:C:392:PHE:CE2	2.81	0.67
2:C:434:THR:HG22	2:C:442:VAL:HG11	1.75	0.67
1:B:365:HIS:CD2	1:B:366:LEU:CD1	2.77	0.67
1:D:34:GLU:HG2	1:D:36:ILE:HG23	1.77	0.67
1:A:268:GLU:OE1	1:A:300:HIS:ND1	2.28	0.67
1:A:268:GLU:CD	1:A:268:GLU:H	1.98	0.67
1:A:450[B]:CYS:CB	4:A:1502:CHT:HC41	1.68	0.67
1:A:162:LEU:O	1:A:166[A]:THR:HG23	1.96	0.66
2:C:321:SER:CB	2:C:325:GLU:OE1	2.41	0.65
2:C:474:GLN:N	2:C:474:GLN:OE1	2.28	0.65
1:B:280:ILE:HG23	1:B:284:PHE:HD2	1.62	0.65
1:A:228:VAL:O	1:A:252:LYS:NZ	2.25	0.65
1:B:303:ILE:O	1:B:306:GLU:OE1	2.14	0.65
1:B:430:CYS:O	1:B:434:THR:HG23	1.97	0.64
1:D:450:CYS:H	6:D:1503:GOL:C3	2.08	0.64
1:B:303:ILE:CA	1:B:306:GLU:OE1	2.45	0.64
1:D:450:CYS:H	6:D:1503:GOL:H32	1.62	0.64
1:B:273:ASP:OD1	1:B:310:LYS:CD	2.45	0.64
1:A:279:THR:HG21	1:A:307:PHE:HZ	1.63	0.63
2:C:455:PRO:O	1:D:481:GLN:NE2	2.31	0.63
2:C:81:LYS:HZ3	2:C:200:GLU:CB	2.02	0.63
1:A:431:GLU:HG3	3:B:1498:IOD:I	2.69	0.63
1:D:362:ARG:NH2	1:D:369:GLY:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:VAL:HB	1:B:275:VAL:HG21	1.80	0.62
1:D:380:ILE:HG13	1:D:397[B]:CYS:HB2	1.82	0.62
2:C:496:SER:O	8:C:2163:HOH:O	2.16	0.62
2:C:228:VAL:O	2:C:252:LYS:HE3	2.00	0.62
1:B:273:ASP:OD1	1:B:310:LYS:HD2	2.00	0.62
1:D:304:ALA:O	1:D:308:VAL:HG12	2.00	0.61
1:A:269:ASP:O	1:A:425:ASN:ND2	2.29	0.60
1:B:365:HIS:CD2	1:B:366:LEU:HD11	2.36	0.60
1:B:291[B]:CSO:SG	4:B:1501:CHT:H82	2.42	0.60
1:B:303:ILE:HA	1:B:306:GLU:OE1	2.02	0.60
2:C:298:LEU:HD21	2:C:387:TRP:HH2	1.67	0.60
1:B:310:LYS:HB2	1:B:310:LYS:NZ	2.17	0.59
1:A:268:GLU:OE1	1:A:268:GLU:N	2.34	0.59
2:C:404:GLU:OE2	2:C:432:ARG:NH2	2.35	0.59
1:A:450[B]:CYS:CB	4:A:1502:CHT:C4	2.44	0.59
2:C:234:THR:HG23	2:C:257[B]:GLU:HG3	1.85	0.59
1:B:5:ILE:HD11	1:B:37:GLY:HA3	1.83	0.59
1:A:63:TRP:O	1:A:66:THR:HG22	2.03	0.58
1:A:273:ASP:OD1	1:A:310:LYS:HE2	2.03	0.58
1:A:320:ILE:HG12	1:A:330:LEU:HD23	1.86	0.58
1:B:365:HIS:C	1:B:366:LEU:HD12	2.23	0.57
2:C:160:TYR:HB2	2:C:164:MET:HG2	1.86	0.57
1:A:301:GLU:HA	1:A:304:ALA:HB2	1.87	0.57
2:C:5:ILE:HD11	2:C:95:ILE:HG21	1.87	0.57
1:B:58:PHE:CE2	1:B:150:GLY:HA2	2.40	0.57
1:D:320:ILE:HD11	1:D:374:PRO:HD3	1.86	0.57
2:C:146[A]:ARG:NH1	8:C:2058:HOH:O	2.38	0.57
1:D:260:GLY:HA2	1:D:416:TYR:CD1	2.39	0.57
1:B:303:ILE:HA	1:B:306:GLU:CD	2.26	0.56
1:B:336:LYS:CG	1:B:370:TYR:OH	2.53	0.56
2:C:430:CYS:O	2:C:434:THR:HG23	2.06	0.56
1:A:51:VAL:HG21	1:A:225:HIS:NE2	2.21	0.56
2:C:158:TRP:CH2	2:C:392:PHE:CE2	2.93	0.56
1:A:474:GLN:HG2	3:A:1501:IOD:I	2.75	0.56
2:C:158:TRP:CH2	2:C:392:PHE:HE2	2.23	0.55
2:C:273:ASP:OD1	2:C:314:TRP:NE1	2.39	0.55
1:D:460:LYS:N	5:D:1502:PG4:H22	2.20	0.55
1:B:225:HIS:O	1:B:252:LYS:NZ	2.39	0.55
2:C:20:ILE:HD12	2:C:45:GLU:HB3	1.86	0.55
1:B:160:TYR:HB2	1:B:164:MET:HG2	1.89	0.55
1:B:268:GLU:HA	1:B:303:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291[A]:CSO:SG	4:D:1501:CHT:H62	2.46	0.55
1:B:135:LEU:HD11	1:B:142:SER:HB2	1.89	0.55
1:B:303:ILE:HA	1:B:306:GLU:OE2	2.06	0.55
2:C:146[A]:ARG:HD3	3:C:1499:IOD:I	2.77	0.55
1:A:167:TRP:HH2	4:A:1502:CHT:HC52	1.71	0.54
2:C:260:GLY:HA2	2:C:416:TYR:CD1	2.43	0.54
2:C:290:ILE:HB	2:C:293:ALA:HB2	1.88	0.54
1:D:142:SER:OG	1:D:483:THR:HG22	2.07	0.54
1:D:160:TYR:OH	4:D:1501:CHT:H81	2.07	0.54
1:D:296:ARG:NH2	1:D:410:LEU:O	2.41	0.54
2:C:25[B]:ILE:HD13	2:C:41:ALA:HB2	1.90	0.54
1:D:330:LEU:HD22	1:D:374:PRO:HG3	1.90	0.54
1:A:274:LYS:HG2	1:B:490:PRO:HA	1.90	0.54
1:B:319:LYS:HG2	1:B:321:SER:OG	2.08	0.54
2:C:63:TRP:O	2:C:66[A]:THR:HG22	2.07	0.54
2:C:253:PRO:HD3	5:D:1502:PG4:C1	2.39	0.53
1:D:139:ARG:HG3	1:D:487:SER:HB3	1.91	0.53
1:A:146:ARG:NH2	8:A:2076:HOH:O	2.40	0.53
1:A:275:VAL:O	1:A:279:THR:HG23	2.08	0.53
1:B:273:ASP:OD1	1:B:310:LYS:HE2	2.08	0.53
1:A:5:ILE:HG12	1:A:6:PRO:N	2.23	0.53
1:B:336:LYS:HD2	1:B:370:TYR:HE1	0.38	0.53
2:C:146[A]:ARG:HG2	2:C:477:LEU:HD13	1.90	0.53
1:A:158:TRP:HD1	1:A:184:SER:HG	1.55	0.52
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.91	0.52
2:C:81:LYS:HD2	2:C:201:VAL:CG1	2.39	0.52
1:A:17:ARG:NH2	8:A:2008:HOH:O	2.42	0.52
1:B:63:TRP:O	1:B:66:THR:HG22	2.10	0.52
2:C:157:PRO:HD2	2:C:164:MET:HB3	1.92	0.52
1:A:268:GLU:OE1	1:A:300:HIS:CG	2.63	0.51
1:B:298:LEU:HD21	1:B:387:TRP:HH2	1.75	0.51
1:B:365:HIS:CG	1:B:366:LEU:HD12	2.45	0.51
1:A:256:LEU:HB3	1:A:258:LEU:HD21	1.92	0.51
1:D:328:CYS:O	1:D:329:ARG:NH1	2.44	0.51
1:B:363:PRO:HG2	1:B:371:TYR:HB3	1.92	0.50
1:D:136:PRO:HG2	1:D:137:MET:H	1.77	0.50
1:D:291[A]:CSO:OD	4:D:1501:CHT:H61	2.10	0.50
1:A:450[B]:CYS:SG	4:A:1502:CHT:C4	2.99	0.50
4:B:1501:CHT:O6	4:B:1501:CHT:H62	2.10	0.50
1:B:143:HIS:CE1	3:B:1498:IOD:I	3.35	0.50
1:B:342:ILE:HD13	1:B:393:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:ARG:HH12	2:C:196[A]:GLU:HB2	1.76	0.49
1:D:160:TYR:CZ	4:D:1501:CHT:H81	2.46	0.49
2:C:339:TYR:OH	2:C:362:ARG:NH1	2.46	0.49
1:D:228:VAL:O	1:D:252:LYS:HE2	2.11	0.49
1:D:488:ASP:OD1	1:D:488:ASP:O	2.30	0.49
1:B:273:ASP:OD1	1:B:310:LYS:CE	2.60	0.49
1:B:345:PHE:HD2	1:B:391:VAL:HG13	1.77	0.49
1:B:358:TYR:CD1	1:B:359:GLY:N	2.81	0.49
2:C:27:VAL:HG13	2:C:38:ASP:N	2.28	0.49
2:C:487:SER:HB2	2:C:489:GLU:HG3	1.94	0.49
1:D:251[A]:VAL:HG12	1:D:251[A]:VAL:O	2.13	0.49
1:B:139[B]:ARG:HG3	1:B:487:SER:HB3	1.93	0.49
1:B:447:SER:C	1:B:449[B]:PRO:HD3	2.32	0.49
2:C:474:GLN:CD	3:C:1499:IOD:I	3.21	0.49
1:D:309:ASP:C	1:D:309:ASP:OD1	2.50	0.49
1:A:377:VAL:HG12	1:A:380:ILE:HD11	1.95	0.49
2:C:9:GLN:OE1	2:C:18:GLU:HG3	2.12	0.49
1:A:359:GLY:HA2	1:A:373:GLU:OE1	2.13	0.49
2:C:320:ILE:HD13	2:C:363:PRO:HG2	1.94	0.49
2:C:450:CSO:OD	8:C:2142:HOH:O	2.18	0.49
1:B:364:GLU:OE2	8:B:2107:HOH:O	2.20	0.49
2:C:271:ASP:CG	2:C:274:LYS:HG2	2.34	0.49
1:D:291[A]:CSO:OD	4:D:1501:CHT:C6	2.61	0.49
1:B:309:ASP:O	1:B:312:VAL:HG22	2.13	0.49
1:B:70:HIS:HE1	8:B:2021:HOH:O	1.95	0.48
1:D:130:LYS:NZ	3:D:1498:IOD:I	3.16	0.48
1:D:223[B]:VAL:O	1:D:252:LYS:NZ	2.38	0.48
1:D:460:LYS:H	5:D:1502:PG4:H22	1.77	0.48
1:B:307:PHE:O	1:B:311:LEU:HB2	2.13	0.48
1:B:471:TRP:O	1:B:474:GLN:HG3	2.13	0.48
1:B:139[A]:ARG:HG3	1:B:487:SER:HB3	1.95	0.48
2:C:54:ALA:HA	2:C:206:GLY:O	2.13	0.48
2:C:139:ARG:HG3	2:C:487:SER:HB3	1.95	0.48
2:C:404:GLU:OE1	2:C:432:ARG:NH1	2.46	0.48
1:D:139:ARG:NH2	1:D:489:GLU:O	2.46	0.48
2:C:185:GLU:HB3	2:C:213:GLY:O	2.13	0.48
1:A:160:TYR:CZ	4:A:1502:CHT:H71	2.48	0.48
2:C:265:VAL:HG22	2:C:422:VAL:HG23	1.94	0.48
2:C:135:LEU:HD11	2:C:142:SER:HB2	1.96	0.48
2:C:320:ILE:HD11	2:C:371:TYR:HD1	1.79	0.48
1:A:115:PHE:CZ	1:A:166[B]:THR:HG23	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:HIS:HE1	3:B:1498:IOD:I	2.67	0.47
1:B:247:ALA:HB1	1:B:252:LYS:HG3	1.96	0.47
1:A:234:THR:HG23	1:A:257[A]:GLU:HB3	1.96	0.47
1:A:167:TRP:CH2	4:A:1502:CHT:HC52	2.49	0.47
1:D:275:VAL:HG22	1:D:423:PHE:CD2	2.49	0.47
1:B:448:GLN:N	1:B:449[B]:PRO:HD3	2.30	0.47
1:A:252:LYS:HB2	1:A:252:LYS:HE2	1.76	0.47
5:D:1502:PG4:H51	5:D:1502:PG4:H72	1.52	0.47
2:C:149:LEU:HD11	5:D:1502:PG4:H32	1.95	0.47
2:C:283:CYS:O	2:C:288:GLY:HA2	2.15	0.47
1:D:362:ARG:NH1	1:D:366:LEU:O	2.46	0.47
2:C:423:PHE:CD2	2:C:445:ASN:HA	2.49	0.47
1:D:95:ILE:HG12	1:D:324:PHE:HZ	1.80	0.47
1:A:274:LYS:HE2	1:B:490:PRO:HD3	1.96	0.47
2:C:43:THR:HG23	2:C:45:GLU:H	1.80	0.47
2:C:81:LYS:NZ	2:C:200:GLU:CA	2.77	0.47
1:D:130:LYS:HG3	1:D:145:LEU:HD21	1.97	0.47
1:A:182:LYS:HE2	1:A:213:GLY:O	2.15	0.46
1:B:296:ARG:HD2	1:B:387:TRP:CE3	2.50	0.46
1:B:312:VAL:HG12	1:B:376:ILE:HD13	1.97	0.46
1:A:21:LYS:NZ	3:A:1500:IOD:I	3.17	0.46
1:B:291[A]:CSO:SG	4:B:1501:CHT:H82	2.55	0.46
1:B:448:GLN:N	1:B:449[B]:PRO:CD	2.78	0.46
1:D:58:PHE:CE1	1:D:150:GLY:HA2	2.51	0.46
1:B:337:GLY:O	1:B:341:LYS:HG2	2.16	0.46
1:B:338:GLN:O	1:B:342:ILE:HG13	2.16	0.46
1:D:135:LEU:HD11	1:D:142:SER:HB2	1.98	0.46
1:B:336:LYS:HG2	1:B:370:TYR:CE1	2.30	0.46
2:C:225:HIS:HB3	2:C:228:VAL:HG23	1.97	0.46
1:D:260:GLY:HA2	1:D:416:TYR:CG	2.50	0.46
1:A:362:ARG:NH1	1:A:369:GLY:O	2.42	0.46
1:B:24:ARG:HD3	1:B:38:ASP:OD2	2.14	0.46
2:C:308:VAL:HA	2:C:311:LEU:HB3	1.98	0.46
1:D:271:ASP:HB3	1:D:274:LYS:HD2	1.98	0.46
1:B:429:ARG:O	1:B:433:ILE:HG12	2.16	0.46
1:D:466:ARG:NH2	5:D:1502:PG4:H62	2.31	0.46
1:B:320:ILE:HG12	1:B:330:LEU:HD23	1.96	0.46
1:A:488:ASP:OD1	1:A:488:ASP:O	2.34	0.45
1:B:336:LYS:HG2	1:B:370:TYR:OH	2.10	0.45
1:D:443:TRP:CZ2	1:D:448:GLN:HA	2.51	0.45
1:B:146[B]:ARG:NH1	3:B:1499:IOD:I	3.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLN:HB3	1:B:17:ARG:O	2.16	0.45
1:B:99:LYS:HB2	1:B:103:GLU:OE1	2.16	0.45
1:B:474:GLN:HA	1:B:477:LEU:HD12	1.98	0.45
2:C:149:LEU:HD11	5:D:1502:PG4:C3	2.47	0.45
1:D:455:PRO:HG3	1:D:471:TRP:CZ3	2.51	0.45
8:C:2153:HOH:O	5:D:1502:PG4:H81	2.16	0.45
1:B:337:GLY:C	1:B:341:LYS:HE2	2.32	0.45
1:B:341:LYS:N	1:B:341:LYS:HD3	2.32	0.45
1:B:365:HIS:CD2	1:B:366:LEU:HD12	2.51	0.45
1:D:5:ILE:HD13	1:D:92:LEU:HD22	1.98	0.45
1:D:76:ARG:NH1	1:D:123:GLU:OE2	2.32	0.45
1:A:260:GLY:HA2	1:A:416:TYR:CG	2.52	0.45
4:D:1501:CHT:H82	4:D:1501:CHT:O6	2.17	0.45
1:A:306:GLU:O	1:A:309:ASP:HB3	2.17	0.44
1:B:108:ILE:HA	1:B:111:VAL:HG13	1.99	0.44
1:D:261:LYS:HG3	1:D:296:ARG:CD	2.48	0.44
2:C:260:GLY:HA2	2:C:416:TYR:CG	2.52	0.44
1:D:471:TRP:O	1:D:474:GLN:HG3	2.17	0.44
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.18	0.44
1:A:429:ARG:O	1:A:433:ILE:HG12	2.18	0.44
2:C:59:ARG:NH2	8:C:2017:HOH:O	2.49	0.44
1:A:438:GLU:C	1:A:459:ILE:HD11	2.37	0.44
1:B:291[B]:CSO:HB2	8:B:2089:HOH:O	2.16	0.44
1:B:297:LEU:HD23	1:B:398:VAL:HG13	1.99	0.44
1:A:188:SER:HB3	1:A:212:THR:HG21	1.99	0.44
1:B:139[B]:ARG:NH2	1:B:489:GLU:O	2.51	0.44
1:B:406:GLU:O	1:B:410:LEU:HD13	2.18	0.44
1:D:95:ILE:HG12	1:D:324:PHE:CZ	2.52	0.44
1:D:377:VAL:HG12	1:D:380:ILE:HD11	1.99	0.44
1:B:308:VAL:O	1:B:312:VAL:HG13	2.18	0.43
1:B:365:HIS:CG	1:B:366:LEU:CD1	3.00	0.43
1:D:484:GLN:HG2	1:D:486:ILE:HG23	2.00	0.43
2:C:115:PHE:CE2	2:C:166:THR:HG23	2.53	0.43
1:D:252:LYS:HB2	1:D:252:LYS:HE3	1.78	0.43
1:B:5:ILE:HD12	1:B:6:PRO:O	2.18	0.43
1:D:264:ILE:HG23	1:D:297:LEU:HA	2.00	0.43
1:A:48:GLU:O	1:A:52:VAL:HG23	2.19	0.43
1:B:291[A]:CSO:HB2	8:B:2089:HOH:O	2.18	0.43
2:C:27:VAL:HG12	2:C:39:ILE:HG12	1.99	0.43
1:B:45:GLU:O	1:B:49:VAL:HG13	2.18	0.43
1:B:296:ARG:NH1	1:B:414[B]:THR:HG21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:O	1:A:253:PRO:HD2	2.19	0.43
1:B:86:LYS:HB3	1:B:86:LYS:HE2	1.83	0.43
2:C:33:GLU:HG3	2:C:369:GLY:HA2	1.99	0.43
4:A:1502:CHT:O6	4:A:1502:CHT:H73	2.18	0.43
1:A:76:ARG:HH12	1:A:123:GLU:CD	2.22	0.43
1:B:33:GLU:OE1	1:B:336:LYS:NZ	2.46	0.43
1:B:41:ALA:HA	1:B:213:GLY:HA2	2.00	0.42
1:B:322:ASP:HA	1:B:371:TYR:OH	2.19	0.42
2:C:3:PHE:HE2	2:C:92:LEU:HD21	1.84	0.42
1:D:35:ILE:HD12	1:D:35:ILE:H	1.84	0.42
1:D:290:ILE:HB	1:D:293:ALA:HB2	2.00	0.42
1:A:58:PHE:CE1	1:A:150:GLY:HA2	2.55	0.42
1:B:99:LYS:HD3	1:B:103:GLU:HB3	2.01	0.42
1:A:419:ALA:HA	1:A:439:VAL:HG13	2.00	0.42
1:B:9:GLN:OE1	1:B:18:GLU:HA	2.19	0.42
1:B:154:LEU:HD22	1:B:168:LYS:HB3	2.02	0.42
1:A:131:ALA:HA	1:A:132:PRO:HD3	1.85	0.42
1:A:361:SER:HB2	8:A:2148:HOH:O	2.20	0.42
1:B:5:ILE:HG12	1:B:36:ILE:O	2.19	0.42
1:B:336:LYS:HA	1:B:339:TYR:HB3	2.00	0.42
2:C:158:TRP:HD1	2:C:184:SER:HG	1.65	0.42
1:D:139:ARG:HH22	1:D:490:PRO:C	2.23	0.42
1:A:204:PRO:HA	1:A:205:PRO:HD3	1.88	0.42
2:C:261:LYS:HE3	2:C:296:ARG:HG3	2.01	0.42
1:B:493:TRP:HD1	1:B:494:TYR:CE1	2.38	0.42
2:C:118:PHE:CE1	2:C:171:PRO:HB3	2.55	0.42
2:C:440:GLY:HA3	2:C:457:GLY:O	2.20	0.42
1:A:47:VAL:HG21	1:A:221:PRO:HB2	2.01	0.42
1:A:157:PRO:HB2	8:A:2083:HOH:O	2.20	0.42
1:B:386:ILE:HG23	1:B:397:CYS:SG	2.60	0.42
2:C:51:VAL:HG21	2:C:225:HIS:NE2	2.35	0.42
1:A:354:ALA:HB2	1:A:384:MET:SD	2.59	0.42
1:A:470:GLU:OE1	8:A:2182:HOH:O	2.21	0.42
1:B:280:ILE:HG23	1:B:284:PHE:CD2	2.50	0.42
2:C:81:LYS:HZ2	2:C:200:GLU:CA	2.31	0.42
1:D:280:ILE:HG23	1:D:284:PHE:HD2	1.85	0.42
1:D:466:ARG:CG	5:D:1502:PG4:H71	2.46	0.42
4:B:1501:CHT:H73	4:B:1501:CHT:HC41	1.83	0.41
1:B:367:LYS:HE3	1:B:367:LYS:HB3	1.69	0.41
2:C:280:ILE:HG21	2:C:318:ILE:HD11	2.02	0.41
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:VAL:HG21	2:C:225:HIS:CE1	2.55	0.41
2:C:415:GLU:HB3	2:C:461:ARG:HG3	2.02	0.41
1:B:329:ARG:HD3	1:B:329:ARG:HA	1.90	0.41
2:C:304:ALA:O	2:C:308:VAL:HG12	2.20	0.41
1:A:352:GLU:O	8:A:2146:HOH:O	2.22	0.41
2:C:154:LEU:HD13	2:C:168:LYS:HB3	2.02	0.41
1:D:276:VAL:O	1:D:280:ILE:HG12	2.21	0.41
1:A:281:PHE:O	1:A:285:TRP:HB3	2.21	0.41
1:B:281:PHE:O	1:B:285:TRP:HB3	2.19	0.41
3:C:1498:IOD:I	1:D:431:GLU:HG3	2.90	0.41
1:D:130:LYS:HG2	1:D:143:HIS:CE1	2.56	0.41
1:B:29:ASN:HB2	1:B:36:ILE:HD13	2.03	0.41
1:A:139:ARG:HG3	1:A:487:SER:HB3	2.03	0.41
1:B:188:SER:HB3	1:B:212:THR:HG21	2.01	0.41
1:B:399:LYS:HE3	1:B:399:LYS:HB3	1.93	0.41
2:C:256:LEU:HB3	2:C:258:LEU:HD21	2.03	0.41
2:C:447:SER:C	2:C:449:PRO:HD3	2.40	0.41
1:A:76:ARG:NH1	1:A:123:GLU:OE2	2.47	0.41
1:A:158:TRP:HD1	1:A:184:SER:OG	2.02	0.41
1:B:305:ALA:HA	1:B:308:VAL:HG22	2.02	0.41
1:B:414[B]:THR:HG22	8:B:2112:HOH:O	2.19	0.41
2:C:122:ALA:O	2:C:125:LEU:HB3	2.20	0.41
2:C:258:LEU:CD1	1:D:251[A]:VAL:HG11	2.51	0.41
2:C:453:GLN:NE2	8:C:2044:HOH:O	2.37	0.41
1:D:281:PHE:O	1:D:285:TRP:HB3	2.21	0.41
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.91	0.41
1:A:146:ARG:HB3	1:A:477:LEU:HD13	2.02	0.40
1:A:230:LYS:HE3	1:A:253:PRO:HB2	2.03	0.40
1:A:29:ASN:HA	1:A:30:PRO:HD2	1.91	0.40
1:A:51:VAL:HG21	1:A:225:HIS:CD2	2.56	0.40
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.56	0.40
1:D:169:ILE:HD11	1:D:181:LEU:HD22	2.04	0.40
1:A:310:LYS:HA	1:A:313:LYS:HB2	2.02	0.40
2:C:14:GLY:O	2:C:199:ASN:ND2	2.44	0.40
1:D:486:ILE:H	1:D:486:ILE:HG13	1.58	0.40
1:A:362:ARG:HA	1:A:363:PRO:HD3	1.97	0.40
1:B:185:GLU:HG2	1:B:186:LEU:N	2.36	0.40
2:C:193:GLU:O	2:C:196[B]:GLU:HB3	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	498/498 (100%)	478 (96%)	19 (4%)	1 (0%)	47	44
1	B	501/498 (101%)	470 (94%)	30 (6%)	1 (0%)	47	44
1	D	498/498 (100%)	478 (96%)	16 (3%)	4 (1%)	19	13
2	C	498/497 (100%)	466 (94%)	29 (6%)	3 (1%)	25	19
All	All	1995/1991 (100%)	1892 (95%)	94 (5%)	9 (0%)	34	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	B	448	GLN
2	C	448	GLN
1	D	448	GLN
1	D	136	PRO
2	C	4	PRO
2	C	417	GLY
1	D	251[A]	VAL
1	D	251[B]	VAL

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	414/410 (101%)	410 (99%)	4 (1%)	76	81
1	B	418/410 (102%)	411 (98%)	7 (2%)	60	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	414/410 (101%)	408 (99%)	6 (1%)	67	72
2	C	413/408 (101%)	408 (99%)	5 (1%)	71	76
All	All	1659/1638 (101%)	1637 (99%)	22 (1%)	76	74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	257[A]	GLU
1	A	257[B]	GLU
1	A	428	GLU
1	B	8[A]	ARG
1	B	8[B]	ARG
1	B	306	GLU
1	B	309	ASP
1	B	310	LYS
1	B	341	LYS
1	B	367	LYS
2	C	60[A]	ARG
2	C	60[B]	ARG
2	C	257[A]	GLU
2	C	257[B]	GLU
2	C	313	LYS
1	D	223[A]	VAL
1	D	223[B]	VAL
1	D	257	GLU
1	D	351	SER
1	D	392	PHE
1	D	487	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	B	70	HIS
1	B	143	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)

6 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	CSO	B	291[B]	1	3,6,7	0.64	0	0,6,8	-	-
1	CSO	D	291[A]	1	3,6,7	0.69	0	0,6,8	-	-
1	CSO	B	291[A]	1	3,6,7	0.64	0	0,6,8	-	-
2	CSO	C	450	2	3,6,7	0.65	0	0,6,8	-	-
2	CSO	C	291	2	3,6,7	0.70	0	0,6,8	-	-
1	CSO	A	291[A]	1	3,6,7	0.69	0	0,6,8	-	-

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	CSO	B	291[B]	1	-	1/1/5/7	-
1	CSO	D	291[A]	1	-	1/1/5/7	-
1	CSO	B	291[A]	1	-	0/1/5/7	-
2	CSO	C	450	2	-	0/1/5/7	-
2	CSO	C	291	2	-	0/1/5/7	-
1	CSO	A	291[A]	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	291[B]	CSO	N-CA-CB-SG
1	A	291[A]	CSO	N-CA-CB-SG
1	D	291[A]	CSO	N-CA-CB-SG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	291[B]	CSO	2	0
1	D	291[A]	CSO	3	0
1	B	291[A]	CSO	2	0
2	C	450	CSO	1	0
2	C	291	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 15 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	PG4	A	1503	-	11,11,12	0.73	0	10,10,11	0.42	0
6	GOL	B	1502	-	5,5,5	0.45	0	5,5,5	0.57	0
4	CHT	D	1501	1	6,6,6	1.97	1 (16%)	8,8,8	1.28	1 (12%)
4	CHT	B	1501	1	6,6,6	2.01	1 (16%)	8,8,8	1.15	1 (12%)
7	ETX	C	1501	-	5,5,5	0.36	0	4,4,4	0.42	0
4	CHT	A	1502	1	6,6,6	2.21	3 (50%)	8,8,8	1.74	2 (25%)
6	GOL	D	1503	-	5,5,5	0.26	0	5,5,5	0.28	0
5	PG4	C	1500	-	11,11,12	0.73	0	10,10,11	0.42	0
5	PG4	D	1502	-	11,11,12	0.76	0	10,10,11	0.60	0

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
5	PG4	A	1503	-	-	7/9/9/10	-
6	GOL	B	1502	-	-	2/4/4/4	-
4	CHT	D	1501	1	-	0/4/4/4	-
4	CHT	B	1501	1	-	0/4/4/4	-
7	ETX	C	1501	-	-	1/3/3/3	-
4	CHT	A	1502	1	-	1/4/4/4	-
6	GOL	D	1503	-	-	0/4/4/4	-
5	PG4	C	1500	-	-	3/9/9/10	-
5	PG4	D	1502	-	-	6/9/9/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1502	CHT	O6-C4	-3.91	1.21	1.42
4	B	1501	CHT	O6-C4	-3.90	1.21	1.42
4	D	1501	CHT	O6-C4	-3.66	1.23	1.42
4	A	1502	CHT	C8-N1	-2.25	1.43	1.50
4	A	1502	CHT	C7-N1	-2.14	1.43	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1502	CHT	C8-N1-C5	3.09	122.55	109.92
4	D	1501	CHT	C8-N1-C5	2.25	119.12	109.92
4	B	1501	CHT	C8-N1-C5	2.08	118.43	109.92
4	A	1502	CHT	O6-C4-C5	2.04	120.68	111.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1502	GOL	O1-C1-C2-O2
5	D	1502	PG4	C5-C6-O4-C7
4	A	1502	CHT	O6-C4-C5-N1
5	C	1500	PG4	O3-C5-C6-O4
6	B	1502	GOL	O1-C1-C2-C3
5	C	1500	PG4	O4-C7-C8-O5
5	D	1502	PG4	C8-C7-O4-C6
7	C	1501	ETX	C1-C2-O2-C3
5	D	1502	PG4	C6-C5-O3-C4
5	A	1503	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
5	D	1502	PG4	O4-C7-C8-O5
5	A	1503	PG4	C5-C6-O4-C7
5	C	1500	PG4	C8-C7-O4-C6
5	A	1503	PG4	C1-C2-O2-C3
5	A	1503	PG4	O2-C3-C4-O3
5	A	1503	PG4	C8-C7-O4-C6
5	A	1503	PG4	C4-C3-O2-C2
5	D	1502	PG4	O3-C5-C6-O4
5	A	1503	PG4	O3-C5-C6-O4
5	D	1502	PG4	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1501	CHT	6	0
4	B	1501	CHT	5	0
4	A	1502	CHT	9	0
6	D	1503	GOL	3	0
5	D	1502	PG4	10	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	494/498 (99%)	0.37	27 (5%)	25	24	18, 34, 63, 103	0
1	B	493/498 (98%)	0.52	33 (6%)	17	17	18, 40, 69, 84	0
1	D	494/498 (99%)	0.36	32 (6%)	18	18	17, 31, 57, 108	0
2	C	493/497 (99%)	0.74	46 (9%)	8	8	21, 41, 59, 105	0
All	All	1974/1991 (99%)	0.50	138 (6%)	16	15	17, 37, 65, 108	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	PHE	8.0
1	A	3	PHE	6.9
2	C	324	PHE	5.5
2	C	427	LEU	5.5
2	C	3	PHE	5.4
2	C	290	ILE	5.2
1	D	136	PRO	5.0
1	A	5	ILE	4.6
1	A	488	ASP	4.3
1	B	336	LYS	4.1
1	B	34	GLU	4.1
1	B	366	LEU	3.9
2	C	82	ILE	3.8
1	D	495	LYS	3.8
2	C	283	CYS	3.7
2	C	273	ASP	3.7
2	C	284	PHE	3.6
2	C	22	LYS	3.6
1	D	283	CYS	3.6
1	B	324	PHE	3.5
1	D	133	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	490	PRO	3.5
1	B	313	LYS	3.5
2	C	105	VAL	3.4
2	C	410	LEU	3.4
1	B	154	LEU	3.4
1	B	353	GLY	3.3
1	A	497	PRO	3.3
1	D	497	PRO	3.2
1	A	4	PRO	3.2
1	B	367	LYS	3.1
1	D	34	GLU	3.1
1	B	368	LYS	3.1
2	C	381	SER	3.1
2	C	488	ASP	3.0
1	D	364	GLU	3.0
2	C	313	LYS	3.0
1	B	283	CYS	2.9
1	B	369	GLY	2.9
1	D	138	GLU	2.9
1	A	348	THR	2.9
2	C	101	PHE	2.9
1	B	321	SER	2.9
2	C	312	VAL	2.9
2	C	272	ILE	2.9
1	D	349	ALA	2.9
1	A	346	ILE	2.8
1	B	208	LEU	2.8
1	B	348	THR	2.8
2	C	351	SER	2.8
2	C	396	LEU	2.8
1	D	4	PRO	2.7
1	B	22	LYS	2.7
2	C	86	LYS	2.7
1	D	494	TYR	2.7
1	A	283	CYS	2.7
2	C	264	ILE	2.7
1	D	284	PHE	2.7
1	B	284	PHE	2.6
1	B	20	ILE	2.6
1	A	487	SER	2.6
1	B	282	GLY	2.6
2	C	282	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	163	LEU	2.5
1	B	402	SER	2.5
1	D	326	GLU	2.5
1	A	324	PHE	2.5
2	C	305	ALA	2.5
1	A	282	GLY	2.5
1	A	380	ILE	2.5
2	C	154	LEU	2.5
1	A	326	GLU	2.5
1	D	134	THR	2.5
1	D	491	TRP	2.4
1	B	311	LEU	2.4
2	C	89	PHE	2.4
2	C	368	LYS	2.4
2	C	18	GLU	2.4
1	A	345	PHE	2.4
1	D	140	PHE	2.4
2	C	392	PHE	2.4
1	A	349	ALA	2.4
1	B	420	ALA	2.4
1	D	154	LEU	2.4
2	C	387	TRP	2.4
1	B	309	ASP	2.3
2	C	326	GLU	2.3
1	B	88	HIS	2.3
2	C	279	THR	2.3
1	D	282	GLY	2.3
1	A	286	THR	2.3
1	D	486	ILE	2.3
1	D	493	TRP	2.3
1	D	350	LYS	2.3
2	C	181	LEU	2.3
1	A	495	LYS	2.3
1	D	368	LYS	2.3
1	B	180	VAL	2.3
1	D	280	ILE	2.3
2	C	210	ILE	2.2
1	D	396	LEU	2.2
2	C	77	ALA	2.2
2	C	180	VAL	2.2
2	C	20	ILE	2.2
2	C	4	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	367	LYS	2.2
1	B	305	ALA	2.2
1	A	364	GLU	2.2
1	D	25[A]	ILE	2.2
1	B	354	ALA	2.2
2	C	60[A]	ARG	2.2
1	D	351	SER	2.1
1	D	383[A]	SER	2.1
2	C	269	ASP	2.1
2	C	189	VAL	2.1
1	D	137	MET	2.1
1	B	155	ILE	2.1
1	D	210	ILE	2.1
2	C	268	GLU	2.1
1	B	370	TYR	2.1
1	B	344	LYS	2.1
1	A	169	ILE	2.1
1	A	419	ALA	2.1
1	B	349	ALA	2.1
1	D	369	GLY	2.1
1	A	456	TRP	2.1
1	D	180	VAL	2.1
1	A	351	SER	2.1
1	B	280	ILE	2.1
1	A	181	LEU	2.1
1	B	315	THR	2.0
1	A	162	LEU	2.0
1	B	181	LEU	2.0
2	C	208	LEU	2.0
2	C	376	ILE	2.0
1	A	395	VAL	2.0
1	A	362	ARG	2.0
2	C	177	CYS	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CSO	C	450	7/8	0.76	0.19	44,54,57,71	0
2	CSO	C	291	7/8	0.90	0.13	31,37,53,59	0
1	CSO	A	291[A]	7/8	0.93	0.15	16,21,34,35	7
1	CSO	B	291[A]	7/8	0.95	0.19	30,30,36,37	7
1	CSO	B	291[B]	7/8	0.95	0.19	30,30,36,37	7
1	CSO	D	291[A]	7/8	0.96	0.16	20,22,30,33	7

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	1502	6/6	0.73	0.19	49,55,56,63	0
7	ETX	C	1501	6/6	0.74	0.20	54,59,69,73	0
6	GOL	D	1503	6/6	0.81	0.23	48,59,61,63	0
5	PG4	D	1502	12/13	0.88	0.17	16,30,43,46	0
4	CHT	D	1501	7/7	0.90	0.42	22,24,31,31	7
5	PG4	A	1503	12/13	0.90	0.15	19,35,41,49	0
4	CHT	A	1502	7/7	0.90	0.34	20,25,33,36	7
4	CHT	B	1501	7/7	0.92	0.31	27,32,36,37	7
3	IOD	A	1500	1/1	0.94	0.08	43,43,43,43	1
5	PG4	C	1500	12/13	0.94	0.12	26,40,53,57	0
3	IOD	D	1500	1/1	0.96	0.08	37,37,37,37	1
3	IOD	B	1499	1/1	0.96	0.08	39,39,39,39	1
3	IOD	B	502	1/1	0.97	0.05	46,46,46,46	1
3	IOD	C	1499	1/1	0.97	0.07	44,44,44,44	1
3	IOD	B	1498	1/1	0.98	0.10	38,38,38,38	1
3	IOD	A	501	1/1	0.98	0.07	41,41,41,41	1
3	IOD	B	1500	1/1	0.98	0.08	53,53,53,53	1
3	IOD	A	1498	1/1	0.98	0.06	49,49,49,49	1
3	IOD	D	1498	1/1	0.98	0.04	42,42,42,42	1
3	IOD	C	503	1/1	0.99	0.05	42,42,42,42	1
3	IOD	C	1498	1/1	0.99	0.06	41,41,41,41	1
3	IOD	A	1499	1/1	0.99	0.08	42,42,42,42	1
3	IOD	A	1501	1/1	0.99	0.05	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IOD	D	1499	1/1	0.99	0.06	43,43,43,43	1

6.5 Other polymers (i)

There are no such residues in this entry.