



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 03:44 PM EST

PDB ID : 4WHQ
Title : Alkylperoxy reaction intermediate trapped in Protocatechuate 3,4-dioxygenase (pseudomonas putida) at pH 6.5
Authors : Knoot, C.J.; Purpero, V.M.; Lipscomb, J.D.
Deposited on : 2014-09-23
Resolution : 1.78 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 ⓘ 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 ⓘ](#)) 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 : 2.36
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) : 2.36

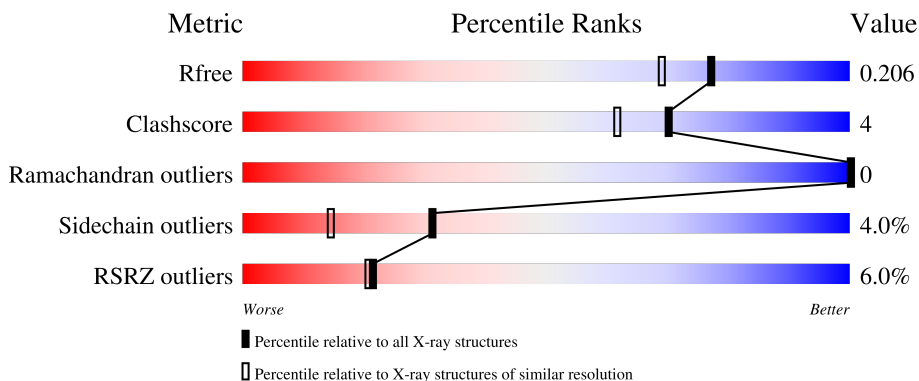
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 $\leq 5\%$. 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	200	
1	C	200	
1	E	200	
2	B	238	
2	D	238	

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Mol	Chain	Length	Quality of chain
2	F	238	 A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a small red segment on the left labeled '5%', a large green segment in the middle labeled '87%', and a small yellow segment on the right labeled '10%'. There are two small black dots at the far right end of the bar.

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 11539 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1581	999	278	301	3	0	1	0
1	E	200	1575	996	277	299	3	0	0	0
1	C	200	1581	999	278	301	3	0	1	0

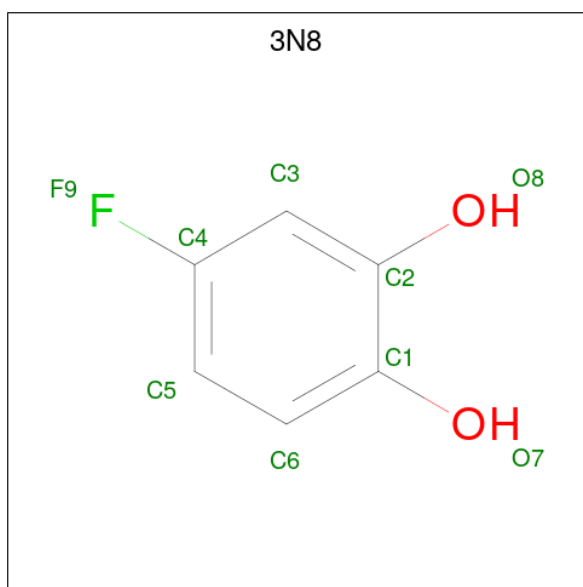
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	236	1889	1200	343	339	7	0	2	0
2	D	238	1902	1208	346	340	8	0	2	0
2	B	238	1894	1202	345	339	8	0	1	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 4-fluorobenzene-1,2-diol (three-letter code: 3N8) (formula: C₆H₅FO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			9	6	1	2		
4	E	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	F	1	Total	C	F	O	0	0
			9	6	1	2		
4	C	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	D	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		

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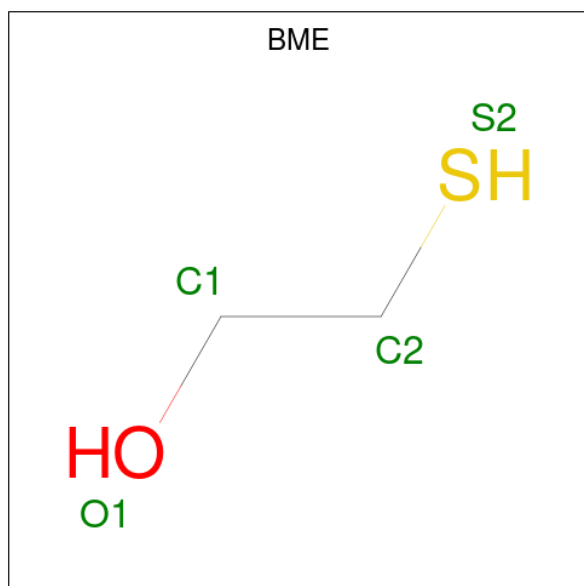
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		
4	B	1	Total	C	F	O	0	0
			9	6	1	2		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		
5	B	1	Total	Fe	0	0
			1	1		

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



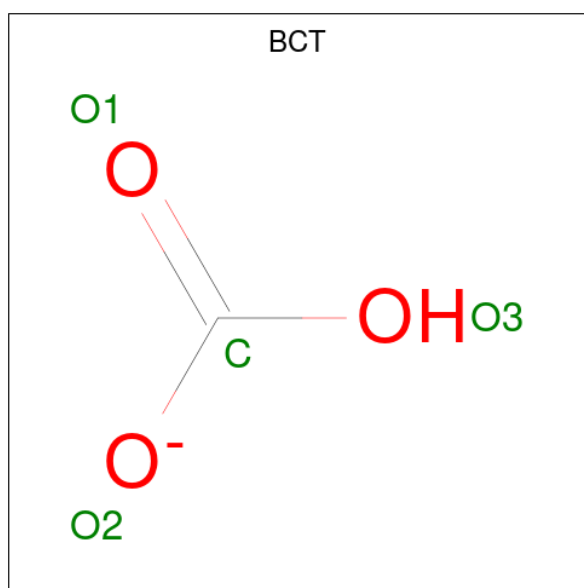
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	S	0	0
			4	2	1	1		
6	F	1	Total	C	O	S	0	0
			4	2	1	1		
6	F	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	D	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	1	3		
7	F	1	Total	C	O	0	0
			4	1	3		
7	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

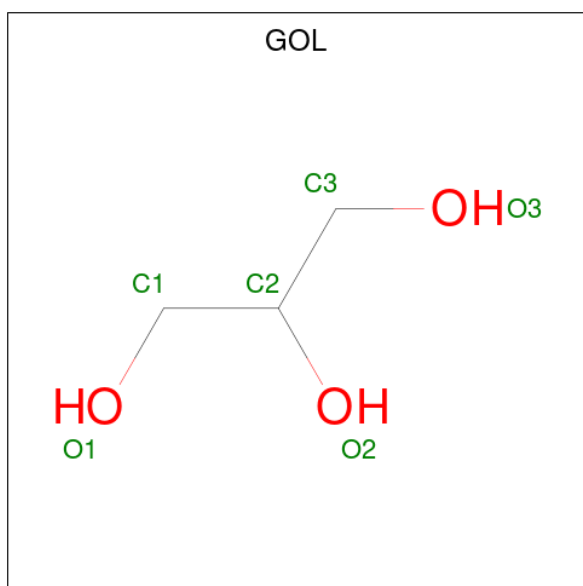


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

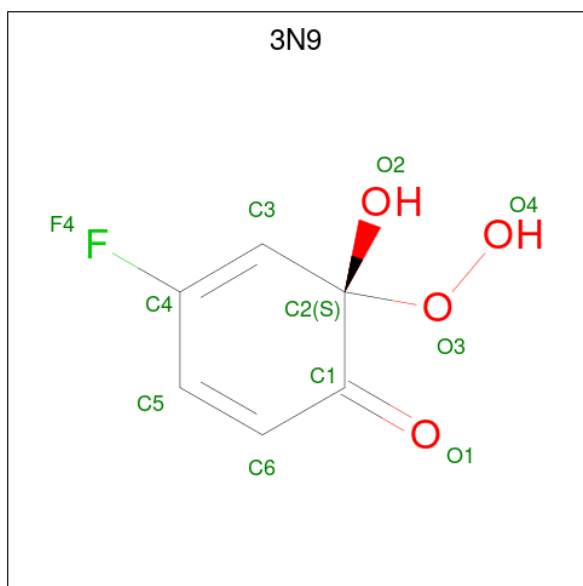
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Na 1 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 11 is (6S)-4-fluoro-6-hydroperoxy-6-hydroxycyclohexa-2,4-dien-1-one (three-letter code: 3N9) (formula: C₆H₅FO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 12 is water.

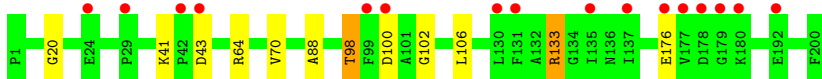
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	127	Total	O	0	0
			127	127		
12	E	96	Total	O	0	0
			96	96		
12	F	166	Total	O	0	0
			166	166		
12	C	141	Total	O	0	0
			141	141		
12	D	182	Total	O	0	0
			182	182		
12	B	179	Total	O	0	0
			179	179		

3 Residue-property plots

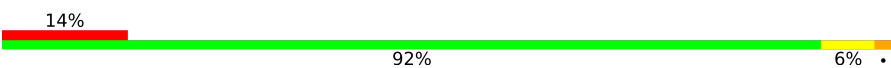
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

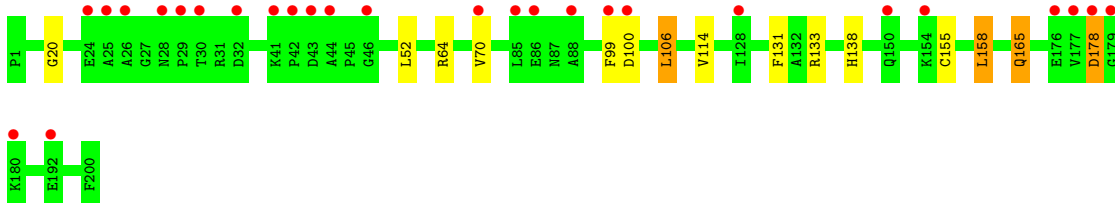
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A: 



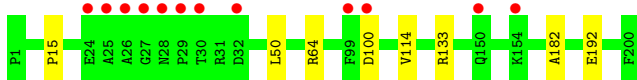
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E: 




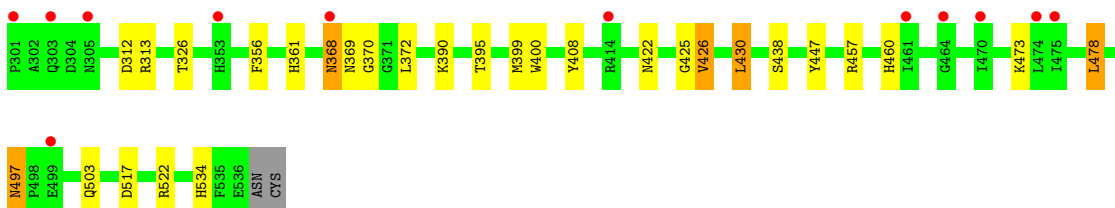
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain C: 

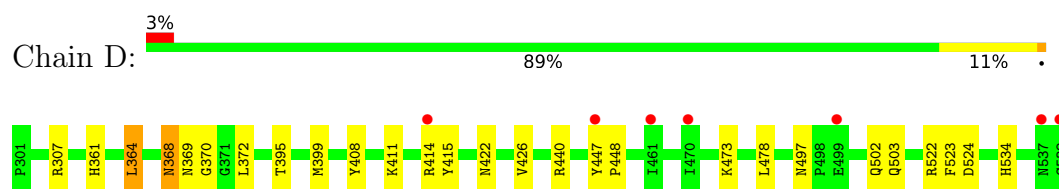


- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

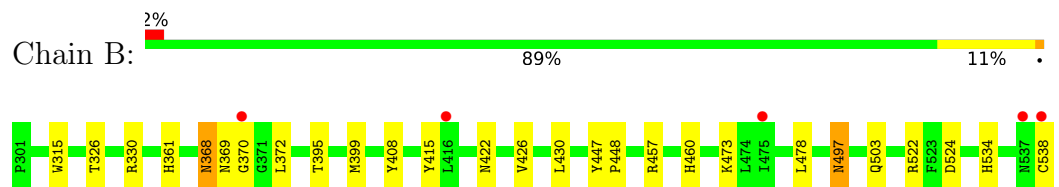
Chain F: 



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.26Å 140.72Å 167.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.78 39.01 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.01-1.78) 97.5 (39.01-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.78Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.195 0.175 , 0.206	Depositor DCC
R_{free} test set	7059 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11539	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, 3N9, 3N8, BME, GOL, FE, SO4, CL, BCT

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	0.57	0/1621	0.76	2/2207 (0.1%)
1	C	0.56	0/1621	0.72	0/2207
1	E	0.53	0/1615	0.71	0/2199
2	B	0.64	0/1951	0.81	3/2657 (0.1%)
2	D	0.59	0/1959	0.77	0/2668
2	F	0.58	0/1945	0.80	6/2647 (0.2%)
All	All	0.58	0/10712	0.77	11/14585 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	133	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	F	426	VAL	CB-CA-C	-6.39	99.26	111.40
2	B	457	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	F	313	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	B	457	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	B	522	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	F	312	ASP	CB-CG-OD1	5.20	122.98	118.30
2	F	457	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	F	522	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	F	517	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1581	0	1514	6	0
1	C	1581	0	1514	3	0
1	E	1575	0	1510	9	0
2	B	1894	0	1846	22	0
2	D	1902	0	1856	23	0
2	F	1889	0	1841	15	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	A	9	0	3	0	0
4	B	54	0	20	0	0
4	C	9	0	4	0	0
4	D	36	0	15	1	0
4	E	9	0	3	0	0
4	F	36	0	13	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	B	12	0	18	2	0
6	C	4	0	6	0	0
6	D	4	0	6	3	0
6	F	12	0	18	0	0
7	B	4	0	0	0	0
7	F	8	0	0	0	0
8	C	5	0	0	1	0
9	D	1	0	0	0	0
10	D	6	0	8	3	0
11	B	11	0	3	3	0
12	A	127	0	0	0	0
12	B	179	0	0	2	1
12	C	141	0	0	0	0
12	D	182	0	0	3	0
12	E	96	0	0	0	0
12	F	166	0	0	0	0
All	All	11539	0	10198	74	1

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 4.

All (74) 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)
2:B:447[B]:TYR:CE1	12:B:870:HOH:O	2.28	0.86
2:D:447[B]:TYR:CE1	12:D:876:HOH:O	2.30	0.84
1:E:20:GLY:HA2	2:F:426:VAL:HG13	1.73	0.71
2:B:447[A]:TYR:OH	11:B:612:3N9:H1	1.91	0.70
2:B:415:TYR:HB2	12:B:870:HOH:O	1.93	0.69
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.75	0.68
2:B:447[A]:TYR:OH	11:B:612:3N9:C3	2.40	0.68
2:B:369:ASN:H	2:B:422:ASN:HD22	1.42	0.68
1:E:70:VAL:HG11	1:E:106:LEU:HD21	1.77	0.66
1:E:165:GLN:H	1:E:165:GLN:HE21	1.42	0.65
2:F:369:ASN:H	2:F:422:ASN:HD22	1.48	0.59
2:D:369:ASN:H	2:D:422:ASN:HD22	1.50	0.59
2:F:447[B]:TYR:CE2	2:F:460:HIS:HE1	2.20	0.59
2:B:447[A]:TYR:HB2	2:B:448:PRO:HD2	1.85	0.58
1:E:64:ARG:NH2	1:E:100:ASP:O	2.36	0.58
2:D:307:ARG:HD2	10:D:608:GOL:C1	2.33	0.58
2:D:364:LEU:HD22	2:D:440:ARG:HG2	1.86	0.57
2:F:368:ASN:ND2	2:F:370:GLY:H	2.05	0.55
2:D:415:TYR:HB2	12:D:876:HOH:O	2.06	0.54
1:A:70:VAL:HG11	1:A:106:LEU:HD11	1.89	0.54
2:F:447[B]:TYR:CE2	2:F:460:HIS:CE1	2.94	0.54
2:B:524:ASP:H	6:B:608:BME:H22	1.72	0.54
1:C:15:PRO:HB3	1:C:133:ARG:HD3	1.91	0.53
2:F:356:PHE:CZ	2:F:430:LEU:HD13	2.44	0.52
2:D:361:HIS:CD2	2:D:361:HIS:H	2.28	0.52
2:B:408:TYR:HE2	2:B:447[A]:TYR:CZ	2.27	0.52
2:D:408:TYR:HE2	2:D:447[A]:TYR:CZ	2.28	0.51
2:D:307:ARG:HD2	10:D:608:GOL:H11	1.91	0.51
2:F:408:TYR:HE2	2:F:447[B]:TYR:CE2	2.28	0.51
1:C:64:ARG:NH1	8:C:304:SO4:O3	2.43	0.51
2:D:478:LEU:C	2:D:478:LEU:HD23	2.32	0.50
2:D:447[A]:TYR:HB2	2:D:448:PRO:HD2	1.94	0.50
1:E:64:ARG:HD3	1:E:99:PHE:O	2.13	0.49
2:B:361:HIS:H	2:B:361:HIS:CD2	2.30	0.49
2:F:361:HIS:H	2:F:361:HIS:CD2	2.31	0.49
2:D:368:ASN:HD22	2:D:368:ASN:C	2.16	0.48
2:B:368:ASN:C	2:B:368:ASN:HD22	2.16	0.48
2:F:408:TYR:CE2	2:F:447[B]:TYR:CE2	3.02	0.47
1:A:64:ARG:NH2	1:A:100:ASP:O	2.48	0.47
2:B:478:LEU:HD23	2:B:478:LEU:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:497:ASN:C	2:F:497:ASN:HD22	2.19	0.47
2:D:524:ASP:H	6:D:606:BME:H12	1.81	0.46
2:D:368:ASN:ND2	2:D:370:GLY:H	2.13	0.46
2:B:447[A]:TYR:CE2	2:B:460:HIS:HE1	2.33	0.46
1:E:133:ARG:HG2	2:F:326:THR:HG21	1.98	0.46
2:F:408:TYR:HE2	2:F:447[B]:TYR:CZ	2.34	0.45
2:D:414:ARG:NE	2:D:414:ARG:HA	2.32	0.45
2:F:478:LEU:C	2:F:478:LEU:HD23	2.37	0.44
2:D:307:ARG:HD2	10:D:608:GOL:H12	1.98	0.44
2:B:408:TYR:HE2	2:B:447[A]:TYR:CE2	2.35	0.44
1:A:133:ARG:HG2	2:B:326:THR:HG21	2.00	0.44
2:B:524:ASP:H	6:B:608:BME:C2	2.30	0.44
2:D:408:TYR:HE2	2:D:447[A]:TYR:CE2	2.35	0.44
2:B:408:TYR:CE2	2:B:447[A]:TYR:CE2	3.06	0.43
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.53	0.43
1:E:155:CYS:HB3	1:E:158:LEU:HB2	2.00	0.43
2:D:447[A]:TYR:O	2:D:447[A]:TYR:CD1	2.71	0.43
2:B:315:TRP:HZ2	2:B:503:GLN:HE21	1.65	0.43
2:D:408:TYR:CE2	2:D:447[A]:TYR:CE2	3.07	0.43
2:D:447[A]:TYR:CD1	2:D:447[A]:TYR:C	2.91	0.43
2:D:503:GLN:HG2	12:D:775:HOH:O	2.18	0.43
2:D:524:ASP:H	6:D:606:BME:C1	2.32	0.43
2:B:326:THR:HG22	2:B:330:ARG:HD2	2.01	0.42
2:B:497:ASN:C	2:B:497:ASN:HD22	2.23	0.42
2:B:368:ASN:ND2	2:B:370:GLY:H	2.17	0.42
1:E:178:ASP:N	1:E:178:ASP:OD1	2.52	0.42
2:D:426:VAL:HG12	4:D:602:3N8:C3	2.50	0.42
1:A:41:LYS:HD2	1:A:88:ALA:HA	2.01	0.41
2:B:408:TYR:CZ	11:B:612:3N9:O4	2.73	0.41
2:F:356:PHE:HZ	2:F:430:LEU:HD13	1.86	0.41
2:F:400:TRP:HA	2:F:425:GLY:O	2.20	0.41
2:D:523:PHE:HA	6:D:606:BME:H11	2.03	0.41
1:C:50:LEU:O	1:C:182:ALA:HA	2.20	0.41
1:A:98:THR:HG22	1:A:102:GLY:N	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:738:HOH:O	12:B:738:HOH:O[2_555]	2.03	0.17

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	199/200 (100%)	194 (98%)	5 (2%)	0	100	100
1	C	199/200 (100%)	194 (98%)	5 (2%)	0	100	100
1	E	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
2	B	237/238 (100%)	229 (97%)	8 (3%)	0	100	100
2	D	238/238 (100%)	231 (97%)	7 (3%)	0	100	100
2	F	235/238 (99%)	231 (98%)	4 (2%)	0	100	100
All	All	1306/1314 (99%)	1272 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	164/163 (101%)	161 (98%)	3 (2%)	59	45
1	C	164/163 (101%)	161 (98%)	3 (2%)	59	45
1	E	163/163 (100%)	157 (96%)	6 (4%)	34	17
2	B	203/202 (100%)	194 (96%)	9 (4%)	28	12
2	D	204/202 (101%)	193 (95%)	11 (5%)	22	8
2	F	202/202 (100%)	190 (94%)	12 (6%)	19	6
All	All	1100/1095 (100%)	1056 (96%)	44 (4%)	31	14

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	98	THR
1	A	176	GLU
1	E	52	LEU
1	E	106	LEU
1	E	114	VAL
1	E	158	LEU
1	E	165	GLN
1	E	178	ASP
2	F	368	ASN
2	F	372	LEU
2	F	390	LYS
2	F	395	THR
2	F	399	MET
2	F	430	LEU
2	F	438	SER
2	F	473	LYS
2	F	478	LEU
2	F	497	ASN
2	F	503	GLN
2	F	534	HIS
1	C	100	ASP
1	C	114	VAL
1	C	192	GLU
2	D	364	LEU
2	D	368	ASN
2	D	372	LEU
2	D	395	THR
2	D	399	MET
2	D	411	LYS
2	D	473	LYS
2	D	497	ASN
2	D	502	GLN
2	D	522	ARG
2	D	534	HIS
2	B	368	ASN
2	B	372	LEU
2	B	395	THR
2	B	399	MET
2	B	430	LEU
2	B	473	LYS
2	B	497	ASN

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Mol	Chain	Res	Type
2	B	534	HIS
2	B	538	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	E	159	ASN
1	E	165	GLN
2	F	361	HIS
2	F	368	ASN
2	F	412	ASN
2	F	422	ASN
2	F	497	ASN
2	F	503	GLN
2	D	361	HIS
2	D	368	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
2	B	361	HIS
2	B	368	ASN
2	B	412	ASN
2	B	422	ASN
2	B	497	ASN
2	B	503	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 7 are monoatomic - leaving 31 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
4	3N8	B	602	-	9,9,9	0.99	0	12,12,12	1.26	2 (16%)
6	BME	F	610	-	3,3,3	0.34	0	1,2,2	0.23	0
4	3N8	D	604	-	9,9,9	0.79	0	12,12,12	0.95	0
7	BCT	B	611	-	2,3,3	0.74	0	2,3,3	0.52	0
4	3N8	D	605	-	9,9,9	0.96	0	12,12,12	0.83	0
6	BME	F	605	-	3,3,3	0.44	0	1,2,2	1.00	0
7	BCT	F	609	-	2,3,3	0.73	0	2,3,3	1.02	0
6	BME	B	609	-	3,3,3	0.26	0	1,2,2	0.25	0
6	BME	B	606	-	3,3,3	0.52	0	1,2,2	0.60	0
4	3N8	B	610	-	9,9,9	0.69	0	12,12,12	0.80	0
4	3N8	F	603	-	9,9,9	0.69	0	12,12,12	0.89	1 (8%)
4	3N8	E	301	-	9,9,9	0.79	0	12,12,12	0.92	0
4	3N8	A	302	-	9,9,9	0.79	0	12,12,12	1.08	1 (8%)
4	3N8	B	605	-	9,9,9	0.84	0	12,12,12	0.86	0
6	BME	C	302	-	3,3,3	0.36	0	1,2,2	0.40	0
10	GOL	D	608	-	5,5,5	0.69	0	5,5,5	1.10	0
6	BME	D	606	-	3,3,3	0.54	0	1,2,2	0.18	0
6	BME	B	608	-	3,3,3	0.46	0	1,2,2	0.72	0
6	BME	F	606	-	3,3,3	0.39	0	1,2,2	0.15	0
7	BCT	F	607	-	2,3,3	0.76	0	2,3,3	1.08	0
4	3N8	D	602	-	9,9,9	1.42	3 (33%)	12,12,12	1.85	3 (25%)
4	3N8	F	602	-	9,9,9	1.05	1 (11%)	12,12,12	1.21	2 (16%)
8	SO4	C	304	-	4,4,4	0.30	0	6,6,6	0.18	0
4	3N8	F	608	-	9,9,9	1.47	2 (22%)	12,12,12	1.79	3 (25%)
4	3N8	D	603	-	9,9,9	0.84	0	12,12,12	1.11	1 (8%)
4	3N8	C	301	-	9,9,9	0.81	0	12,12,12	0.93	0
4	3N8	B	604	-	9,9,9	0.69	0	12,12,12	0.80	0
4	3N8	B	603	-	9,9,9	0.82	0	12,12,12	1.12	2 (16%)
11	3N9	B	612	-	8,11,11	3.07	4 (50%)	3,16,16	2.40	1 (33%)
4	3N8	B	607	-	9,9,9	0.67	0	12,12,12	1.15	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3N8	F	604	-	9,9,9	0.84	0	12,12,12	0.88	1 (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
4	3N8	B	602	-	-	-	0/1/1/1
6	BME	F	610	-	-	0/1/1/1	-
4	3N8	D	604	-	-	-	0/1/1/1
4	3N8	D	605	-	-	-	0/1/1/1
6	BME	F	605	-	-	0/1/1/1	-
6	BME	B	609	-	-	0/1/1/1	-
6	BME	B	606	-	-	1/1/1/1	-
4	3N8	B	610	-	-	-	0/1/1/1
4	3N8	F	603	-	-	-	0/1/1/1
4	3N8	E	301	-	-	-	0/1/1/1
4	3N8	A	302	-	-	-	0/1/1/1
4	3N8	B	605	-	-	-	0/1/1/1
6	BME	C	302	-	-	1/1/1/1	-
10	GOL	D	608	-	-	3/4/4/4	-
6	BME	D	606	-	-	0/1/1/1	-
6	BME	B	608	-	-	1/1/1/1	-
6	BME	F	606	-	-	1/1/1/1	-
4	3N8	D	602	-	-	-	0/1/1/1
4	3N8	F	602	-	-	-	0/1/1/1
4	3N8	F	608	-	-	-	0/1/1/1
4	3N8	D	603	-	-	-	0/1/1/1
4	3N8	C	301	-	-	-	0/1/1/1
4	3N8	B	604	-	-	-	0/1/1/1
11	3N9	B	612	-	-	0/0/19/19	0/1/1/1
4	3N8	B	603	-	-	-	0/1/1/1
4	3N8	B	607	-	-	-	0/1/1/1
4	3N8	F	604	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	612	3N9	C2-C1	-5.08	1.48	1.55
11	B	612	3N9	C6-C1	-4.71	1.38	1.46
11	B	612	3N9	C2-C3	-4.64	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	608	3N8	C3-C4	2.85	1.42	1.37
4	D	602	3N8	C3-C4	2.55	1.42	1.37
4	F	608	3N8	C5-C4	2.31	1.41	1.37
4	F	602	3N8	C3-C4	2.23	1.41	1.37
4	D	602	3N8	C5-C4	2.22	1.41	1.37
11	B	612	3N9	C6-C5	2.10	1.40	1.35
4	D	602	3N8	C3-C2	2.09	1.41	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	3N8	C5-C4-C3	-4.24	117.78	123.29
4	F	608	3N8	C5-C4-C3	-3.92	118.20	123.29
11	B	612	3N9	O3-C2-C3	-3.78	99.12	109.58
4	D	602	3N8	C6-C5-C4	3.34	121.82	118.36
4	F	608	3N8	F9-C4-C3	3.12	122.71	118.25
4	D	602	3N8	F9-C4-C3	2.69	122.09	118.25
4	F	608	3N8	C6-C5-C4	2.61	121.06	118.36
4	F	602	3N8	F9-C4-C3	2.45	121.76	118.25
4	B	607	3N8	C5-C4-C3	-2.42	120.14	123.29
4	F	602	3N8	C5-C4-C3	-2.41	120.16	123.29
4	B	602	3N8	C5-C4-C3	-2.19	120.44	123.29
4	B	603	3N8	C5-C4-C3	-2.18	120.47	123.29
4	B	603	3N8	F9-C4-C3	2.08	121.23	118.25
4	D	603	3N8	C5-C4-C3	-2.05	120.63	123.29
4	F	604	3N8	C6-C1-C2	2.04	121.91	119.67
4	A	302	3N8	C3-C2-C1	2.03	121.66	119.86
4	B	602	3N8	F9-C4-C3	2.02	121.13	118.25
4	F	603	3N8	C5-C4-C3	-2.00	120.69	123.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	606	BME	O1-C1-C2-S2
6	C	302	BME	O1-C1-C2-S2
10	D	608	GOL	O1-C1-C2-C3
10	D	608	GOL	O1-C1-C2-O2
6	B	606	BME	O1-C1-C2-S2
6	B	608	BME	O1-C1-C2-S2
10	D	608	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	608	GOL	3	0
6	D	606	BME	3	0
6	B	608	BME	2	0
4	D	602	3N8	1	0
8	C	304	SO4	1	0
11	B	612	3N9	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/200 (100%)	0.25	16 (8%) 12 11	17, 25, 42, 65	0
1	C	200/200 (100%)	0.25	12 (6%) 21 21	17, 25, 41, 56	0
1	E	200/200 (100%)	0.64	27 (13%) 3 3	19, 33, 53, 77	0
2	B	238/238 (100%)	0.01	5 (2%) 63 63	18, 22, 36, 58	0
2	D	238/238 (100%)	0.03	7 (2%) 51 50	18, 22, 34, 60	0
2	F	236/238 (99%)	0.08	12 (5%) 28 26	19, 24, 37, 59	0
All	All	1312/1314 (99%)	0.19	79 (6%) 21 21	17, 24, 42, 77	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	538	CYS	6.0
1	E	177	VAL	6.0
1	E	178	ASP	5.7
2	F	301	PRO	5.1
1	A	178	ASP	4.9
1	E	99	PHE	4.6
1	A	177	VAL	4.3
1	A	24	GLU	4.1
1	E	179	GLY	3.9
1	C	99	PHE	3.8
1	E	100	ASP	3.7
2	F	353	HIS	3.6
1	E	43	ASP	3.5
1	E	176	GLU	3.5
1	C	29	PRO	3.5
1	E	42	PRO	3.5
1	C	25	ALA	3.4
2	D	537	ASN	3.3
1	E	25	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	538	CYS	3.2
1	E	150	GLN	3.2
1	A	99	PHE	3.2
1	A	179	GLY	3.2
1	E	32	ASP	3.1
1	C	32	ASP	3.1
1	E	29	PRO	3.1
1	E	180	LYS	3.1
1	A	100	ASP	3.1
1	C	27	GLY	3.1
2	F	470	ILE	3.0
1	E	128	ILE	3.0
2	D	470	ILE	3.0
2	F	414	ARG	3.0
2	B	537	ASN	2.9
1	C	24	GLU	2.9
1	E	30	THR	2.9
2	B	416	LEU	2.9
1	E	86	GLU	2.9
1	A	43	ASP	2.8
1	A	42	PRO	2.8
1	C	30	THR	2.7
1	A	131	PHE	2.7
2	F	475	ILE	2.6
2	B	475	ILE	2.6
1	A	180	LYS	2.6
1	A	176	GLU	2.6
1	E	192	GLU	2.6
1	A	29	PRO	2.6
2	B	370	GLY	2.5
1	A	192	GLU	2.5
1	C	150	GLN	2.5
2	D	414	ARG	2.4
1	E	44	ALA	2.4
1	E	85	LEU	2.3
1	C	28	ASN	2.3
2	F	305	ASN	2.3
1	E	24	GLU	2.2
1	A	130	LEU	2.2
1	E	41	LYS	2.2
1	A	137	ILE	2.2
2	F	461	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	26	ALA	2.2
2	F	474	LEU	2.2
1	C	100	ASP	2.2
1	C	154	LYS	2.2
1	E	88	ALA	2.2
1	E	70	VAL	2.2
1	A	135	ILE	2.1
2	F	499	GLU	2.1
1	E	46	GLY	2.1
2	D	499	GLU	2.1
2	F	464	GLY	2.1
2	D	447[A]	TYR	2.1
1	E	154	LYS	2.1
1	C	26	ALA	2.0
2	F	303	GLN	2.0
2	D	461	ILE	2.0
1	E	28	ASN	2.0
2	F	368	ASN	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 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	BME	D	606	4/4	0.42	0.22	42,47,48,61	0
6	BME	F	610	4/4	0.56	0.21	39,46,50,65	0
6	BME	B	608	4/4	0.59	0.17	42,44,44,58	0
6	BME	B	606	4/4	0.74	0.19	46,50,52,58	0
4	3N8	D	605	9/9	0.78	0.27	49,50,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	3N8	B	605	9/9	0.78	0.19	39,41,49,54	0
6	BME	F	605	4/4	0.83	0.23	40,41,42,48	0
4	3N8	F	608	9/9	0.85	0.21	36,43,45,46	0
4	3N8	B	607	9/9	0.86	0.32	53,56,59,66	0
4	3N8	D	604	9/9	0.86	0.13	43,44,46,58	0
10	GOL	D	608	6/6	0.86	0.18	46,47,49,50	0
7	BCT	F	609	4/4	0.87	0.19	48,48,49,50	0
4	3N8	F	602	9/9	0.87	0.24	33,39,44,49	0
4	3N8	D	602	9/9	0.88	0.26	33,41,45,46	0
6	BME	F	606	4/4	0.88	0.14	60,60,61,62	0
4	3N8	B	602	9/9	0.88	0.12	38,41,44,50	0
4	3N8	B	610	9/9	0.88	0.24	52,55,57,60	0
4	3N8	B	603	9/9	0.89	0.15	42,44,46,54	0
4	3N8	B	604	9/9	0.89	0.23	32,36,42,50	0
4	3N8	D	603	9/9	0.89	0.23	31,34,40,48	0
4	3N8	F	603	9/9	0.89	0.14	42,43,47,58	0
9	NA	D	607	1/1	0.89	0.09	37,37,37,37	0
6	BME	C	302	4/4	0.89	0.11	41,45,49,62	0
7	BCT	B	611	4/4	0.90	0.24	58,58,62,64	0
4	3N8	F	604	9/9	0.91	0.10	40,44,49,53	0
4	3N8	C	301	9/9	0.92	0.22	34,37,37,42	0
4	3N8	E	301	9/9	0.92	0.13	39,39,42,49	0
8	SO4	C	304	5/5	0.93	0.21	48,60,65,66	0
3	CL	C	303	1/1	0.93	0.06	64,64,64,64	0
6	BME	B	609	4/4	0.93	0.15	31,41,41,48	0
11	3N9	B	612	11/11	0.93	0.28	27,33,36,37	11
7	BCT	F	607	4/4	0.94	0.18	50,50,54,55	0
4	3N8	A	302	9/9	0.95	0.12	28,31,32,36	0
3	CL	A	303	1/1	0.97	0.08	49,49,49,49	0
3	CL	A	301	1/1	0.97	0.05	57,57,57,57	0
5	FE	B	601	1/1	0.99	0.08	21,21,21,21	1
5	FE	D	601	1/1	0.99	0.07	21,21,21,21	1
5	FE	F	601	1/1	1.00	0.07	22,22,22,22	1

6.5 Other polymers [i](#)

There are no such residues in this entry.