



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 2B1X / pdb_00002b1x
Title : Crystal structure of naphthalene 1,2-dioxygenase from *Rhodococcus* sp.
Authors : Gakhar, L.; Malik, Z.A.; Allen, C.C.; Lipscomb, D.A.; Larkin, M.J.; Ramaswamy, S.
Deposited on : 2005-09-16
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

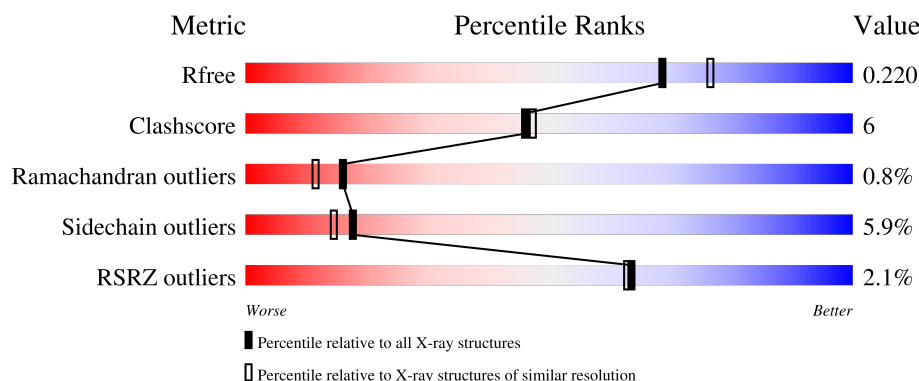
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	470	82% 9% 6%
1	C	470	3% 82% 9% 6%
1	E	470	82% 9% 6%
2	B	172	2% 80% 14% 6%
2	D	172	4% 79% 13% 6%

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Mol	Chain	Length	Quality of chain
2	F	172	3% 78% 15% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15793 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 naphthalene dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			
1	C	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			
1	E	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			

- Molecule 2 is a protein called naphthalene dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			
2	D	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			
2	F	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

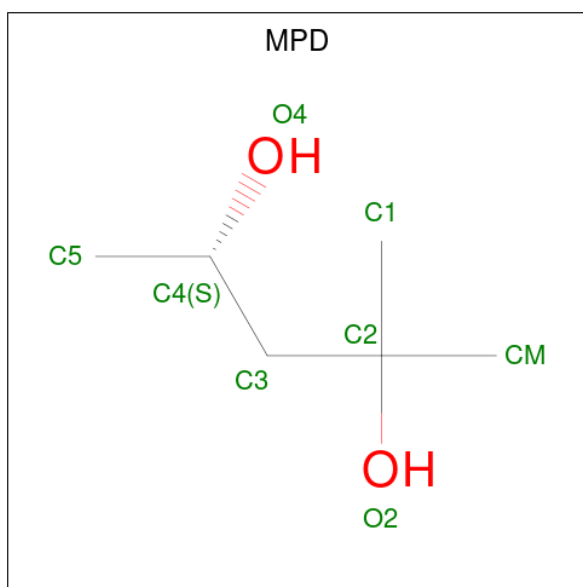
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0

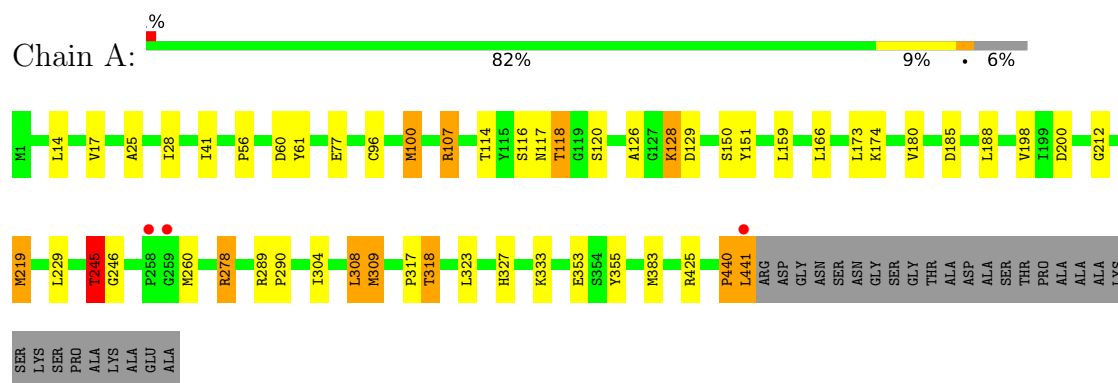
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	253	Total O 253 253	0	0
6	B	95	Total O 95 95	0	0
6	C	251	Total O 251 251	0	0
6	D	109	Total O 109 109	0	0
6	E	298	Total O 298 298	0	0
6	F	106	Total O 106 106	0	0

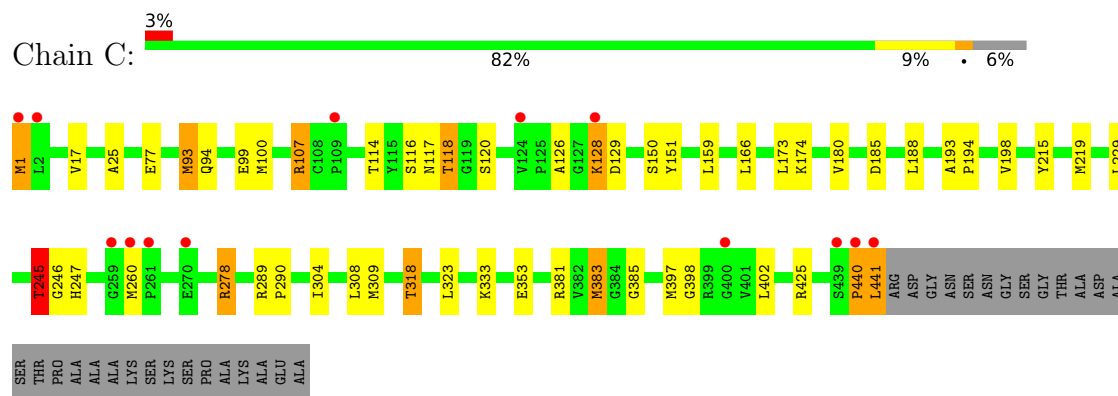
3 Residue-property plots

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.

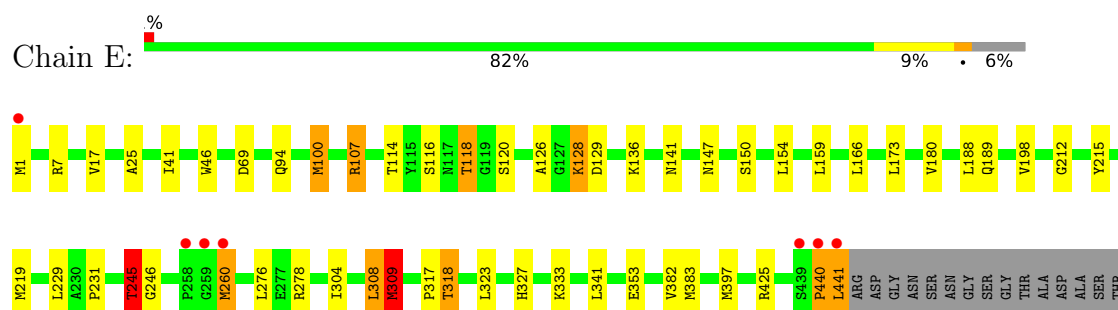
- Molecule 1: naphthalene dioxygenase large subunit



- Molecule 1: naphthalene dioxygenase large subunit



- Molecule 1: naphthalene dioxygenase large subunit



PRO
ALA
ALA
ALA
LYS
SER
LYS
SER
PRO
ALA
LYS
ALA
GLU
ALA

- Molecule 2: naphthalene dioxygenase small subunit

Chain B:  2% 80% 14% . . .

MET ASN THR GLN THR R513 R514 S515 D516 T517 T518 V519 L533 T546 E547 D548 V552 V557 E560 D566 T572 H573 M574 D575 W594 V606 T607 N608 E617 D618 E619 L627 V640 L649 R650 L657 M658 A659 M679

- Molecule 2: naphthalene dioxygenase small subunit

Chain D:  4% 79% 13% . . .

MET ASN THR GLN THR R513 R514 S515 D516 T517 T518 V519 L533 T546 E547 D548 V552 V557 T558 D566 T572 H573 M574 D575 W594 V606 T607 N608 E617 D618 E619 V622 L627 V640 L649 R650 D654 L657 M658 A659 M679

- Molecule 2: naphthalene dioxygenase small subunit

Chain F:  3% 78% 15% . . .

MET ASN THR GLN THR R513 R514 S515 D516 T517 T518 V519 L533 T546 E547 D548 V552 V557 D566 T572 H573 M574 D575 W594 S602 V606 T607 N608 S616 E617 D618 E619 L627 L628 Y629 V640 E644 L649 R650 L657 M658 A659 M679

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.74Å 144.25Å 186.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.80 – 2.00 20.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.80-2.00) 92.8 (20.80-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.224 0.221 , 0.220	Depositor DCC
R_{free} test set	2949 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15793	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FE, MPD

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	0.83	2/3620 (0.1%)	0.93	2/4919 (0.0%)
1	C	0.83	3/3620 (0.1%)	0.92	1/4919 (0.0%)
1	E	0.93	2/3620 (0.1%)	0.96	1/4919 (0.0%)
2	B	0.84	0/1360	0.99	2/1845 (0.1%)
2	D	0.92	2/1360 (0.1%)	1.02	2/1845 (0.1%)
2	F	0.88	1/1360 (0.1%)	1.02	1/1845 (0.1%)
All	All	0.87	10/14940 (0.1%)	0.96	9/20292 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	583	MET	SD-CE	-8.12	1.59	1.79
2	D	574	MET	SD-CE	-7.50	1.60	1.79
1	C	383	MET	SD-CE	-7.00	1.62	1.79
1	E	100	MET	SD-CE	-6.60	1.63	1.79
1	E	309	MET	SD-CE	-6.36	1.63	1.79
1	C	1	MET	SD-CE	5.55	1.93	1.79
1	A	100	MET	SD-CE	-5.50	1.65	1.79
1	A	219	MET	SD-CE	-5.43	1.66	1.79
2	F	574	MET	SD-CE	-5.11	1.66	1.79
1	C	93	MET	CG-SD	-5.10	1.68	1.80

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	245	THR	N-CA-CB	-7.11	100.11	111.62
2	D	572	THR	N-CA-CB	-7.06	99.86	111.66
2	F	572	THR	N-CA-CB	-6.48	100.84	111.66
2	D	552	VAL	N-CA-C	6.45	118.08	108.46
1	A	245	THR	N-CA-CB	-6.22	100.93	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	552	VAL	N-CA-C	6.06	117.49	108.46
2	B	572	THR	N-CA-CB	-6.01	101.62	111.66
1	C	245	THR	N-CA-CB	-5.97	101.95	111.62
1	A	28	ILE	N-CA-C	5.03	115.70	110.82

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	3514	0	3344	33	0
1	C	3514	0	3344	37	0
1	E	3514	0	3344	46	0
2	B	1340	0	1307	21	0
2	D	1340	0	1307	21	0
2	F	1340	0	1307	20	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
4	E	4	0	0	0	0
5	A	32	0	56	0	0
5	C	24	0	42	5	0
5	E	48	0	84	3	0
6	A	253	0	0	2	0
6	B	95	0	0	1	0
6	C	251	0	0	3	0
6	D	109	0	0	0	0
6	E	298	0	0	11	0
6	F	106	0	0	1	0
All	All	15793	0	14135	167	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 (167) 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:572:THR:HG21	2:B:575:ASP:HB2	1.45	0.98
2:F:572:THR:HG21	2:F:575:ASP:HB2	1.43	0.98
2:D:572:THR:HG21	2:D:575:ASP:HB2	1.46	0.96
2:B:608:ASN:HD21	2:F:606:VAL:H	1.26	0.84
1:E:128:LYS:HD2	1:E:129:ASP:H	1.42	0.81
5:C:1707:MPD:H13	1:E:94:GLN:OE1	1.81	0.81
1:A:118:THR:HG22	1:A:120:SER:H	1.46	0.80
1:A:128:LYS:HD2	1:A:129:ASP:H	1.47	0.79
1:C:118:THR:HG22	1:C:120:SER:H	1.47	0.77
1:E:118:THR:HG22	1:E:120:SER:H	1.51	0.76
2:F:619:GLU:HG2	2:F:650:ARG:HG2	1.67	0.76
2:D:619:GLU:HG2	2:D:650:ARG:HG2	1.66	0.75
1:E:128:LYS:CD	1:E:129:ASP:H	1.99	0.75
2:B:606:VAL:H	2:D:608:ASN:HD21	1.34	0.74
2:D:606:VAL:H	2:F:608:ASN:HD21	1.34	0.74
1:E:141:ASN:HB2	6:E:1829:HOH:O	1.86	0.74
2:B:619:GLU:HG2	2:B:650:ARG:HG2	1.69	0.74
1:E:100:MET:HE2	2:F:557:VAL:HG21	1.70	0.73
1:E:107:ARG:HD2	1:E:114:THR:OG1	1.87	0.73
1:C:128:LYS:HD2	1:C:129:ASP:H	1.54	0.71
1:E:219:MET:HE3	1:E:219:MET:HA	1.72	0.70
1:C:100:MET:HE2	2:D:557:VAL:HG21	1.72	0.70
1:A:219:MET:HE2	2:B:594:TRP:HZ2	1.58	0.69
2:F:572:THR:HG23	2:F:574:MET:H	1.58	0.68
1:E:189:GLN:HB2	6:E:1740:HOH:O	1.94	0.68
2:D:546:THR:HG23	2:D:548:ASP:OD1	1.94	0.68
2:F:547:GLU:H	2:F:547:GLU:CD	2.02	0.67
1:A:100:MET:HE2	2:B:557:VAL:HG21	1.75	0.67
1:E:118:THR:HG21	6:E:1874:HOH:O	1.94	0.67
1:A:128:LYS:CD	1:A:129:ASP:H	2.09	0.65
1:C:219:MET:HE3	1:C:219:MET:HA	1.78	0.65
1:A:107:ARG:HD2	1:A:114:THR:OG1	1.97	0.65
1:C:25:ALA:HB1	1:C:383:MET:CE	2.27	0.65
1:A:304:ILE:HG12	1:A:323:LEU:HD22	1.79	0.65
1:A:185:ASP:OD2	1:A:278:ARG:NH2	2.29	0.64
1:C:128:LYS:CD	1:C:129:ASP:H	2.11	0.64
1:C:107:ARG:HD2	1:C:114:THR:OG1	1.98	0.63
2:B:547:GLU:H	2:B:547:GLU:CD	2.08	0.62
1:C:304:ILE:HG12	1:C:323:LEU:HD22	1.81	0.62
1:C:219:MET:HE2	2:D:594:TRP:HZ2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ALA:HB1	1:E:383:MET:CE	2.29	0.62
1:E:128:LYS:HD2	1:E:128:LYS:H	1.63	0.62
2:D:546:THR:CG2	2:D:548:ASP:OD1	2.49	0.61
2:B:515:SER:HB3	2:B:518:THR:HB	1.83	0.60
2:D:547:GLU:CD	2:D:547:GLU:H	2.08	0.60
1:A:219:MET:HA	1:A:219:MET:HE3	1.82	0.60
1:C:381:ARG:HH11	5:C:1707:MPD:H11	1.67	0.60
1:C:17:VAL:O	1:C:425:ARG:HD2	2.01	0.59
1:E:126:ALA:HA	1:E:128:LYS:HE2	1.84	0.59
1:C:25:ALA:HB1	1:C:383:MET:HE2	1.84	0.58
1:E:128:LYS:CD	1:E:128:LYS:H	2.16	0.57
1:E:116:SER:OG	1:E:118:THR:HB	2.03	0.57
2:F:515:SER:HB3	2:F:518:THR:HB	1.85	0.57
1:E:231:PRO:HB3	5:E:1712:MPD:H13	1.87	0.57
1:E:189:GLN:CB	6:E:1740:HOH:O	2.53	0.56
1:C:185:ASP:OD2	1:C:278:ARG:NH2	2.37	0.56
2:B:546:THR:CG2	2:B:659:ALA:HA	2.36	0.55
1:A:383:MET:HA	1:A:383:MET:HE3	1.88	0.55
1:C:77:GLU:HG2	1:C:117:ASN:HD21	1.71	0.55
2:F:627:LEU:HD13	2:F:640:VAL:HG13	1.88	0.55
1:E:308:LEU:HD22	1:E:317:PRO:HB2	1.88	0.55
1:E:318:THR:HG23	6:E:1720:HOH:O	2.04	0.55
2:D:627:LEU:HD13	2:D:640:VAL:HG13	1.89	0.55
1:C:381:ARG:HD3	5:C:1707:MPD:H12	1.89	0.55
1:E:304:ILE:HG12	1:E:323:LEU:HD22	1.88	0.55
2:F:546:THR:HG23	2:F:548:ASP:OD1	2.07	0.54
2:D:515:SER:HB3	2:D:518:THR:HB	1.88	0.54
2:F:619:GLU:OE2	2:F:650:ARG:HD3	2.08	0.54
1:E:17:VAL:O	1:E:425:ARG:HD2	2.08	0.54
1:E:219:MET:HE2	2:F:594:TRP:HZ2	1.74	0.53
1:A:198:VAL:HG11	1:A:333:LYS:HE3	1.90	0.53
1:E:7:ARG:NH2	6:E:1980:HOH:O	2.42	0.53
1:A:25:ALA:HB1	1:A:383:MET:CE	2.39	0.52
1:E:215:TYR:CD2	1:E:397:MET:HE1	2.44	0.52
1:E:327:HIS:HD2	6:E:1725:HOH:O	1.92	0.52
1:E:128:LYS:HD2	1:E:129:ASP:N	2.20	0.52
2:B:515:SER:HB2	2:B:519:VAL:HG23	1.92	0.52
1:E:25:ALA:HB1	1:E:383:MET:HE2	1.91	0.52
1:E:128:LYS:HD2	1:E:128:LYS:N	2.25	0.52
1:C:318:THR:HG23	6:C:1715:HOH:O	2.09	0.52
1:C:99:GLU:HG3	2:D:558:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:THR:HG22	1:E:246:GLY:O	2.10	0.51
1:A:126:ALA:HA	1:A:128:LYS:HE2	1.92	0.51
2:F:572:THR:HG23	2:F:574:MET:N	2.23	0.51
2:B:546:THR:HG23	2:B:548:ASP:OD1	2.11	0.50
1:C:318:THR:HG21	1:C:353:GLU:HB3	1.91	0.50
2:F:546:THR:HG23	2:F:548:ASP:H	1.75	0.50
2:B:546:THR:HG21	2:B:659:ALA:HA	1.92	0.50
1:A:318:THR:HG23	6:A:1714:HOH:O	2.10	0.50
1:C:128:LYS:HD2	1:C:128:LYS:H	1.75	0.50
2:F:557:VAL:O	2:F:566:ASP:HB2	2.11	0.50
1:A:151:TYR:CE2	1:A:174:LYS:HD2	2.47	0.50
1:C:318:THR:CG2	6:C:1715:HOH:O	2.60	0.49
1:A:128:LYS:HD2	1:A:128:LYS:H	1.78	0.49
2:F:644:GLU:OE1	6:F:715:HOH:O	2.20	0.49
1:E:46:TRP:CH2	1:E:147:ASN:HB3	2.48	0.49
2:D:546:THR:HG23	2:D:548:ASP:H	1.78	0.48
1:A:77:GLU:HG2	1:A:117:ASN:HD21	1.78	0.48
2:B:572:THR:HG23	2:B:574:MET:H	1.77	0.48
2:F:515:SER:HB2	2:F:519:VAL:HG23	1.96	0.48
1:A:309:MET:HE2	1:A:309:MET:HB2	1.68	0.48
1:E:260:MET:HE1	5:E:1712:MPD:O2	2.14	0.48
1:A:128:LYS:CD	1:A:128:LYS:H	2.27	0.48
2:D:515:SER:HB2	2:D:519:VAL:HG23	1.96	0.48
1:E:107:ARG:CD	1:E:114:THR:OG1	2.60	0.48
1:A:327:HIS:HD2	6:A:1959:HOH:O	1.97	0.47
1:C:107:ARG:HH12	5:C:1701:MPD:HM1	1.79	0.47
1:C:128:LYS:CD	1:C:128:LYS:H	2.26	0.47
2:D:619:GLU:OE2	2:D:650:ARG:HD3	2.15	0.47
2:D:546:THR:CG2	2:D:659:ALA:HA	2.45	0.47
1:C:126:ALA:HA	1:C:128:LYS:HE2	1.97	0.47
2:D:572:THR:HG23	2:D:574:MET:H	1.79	0.46
1:A:308:LEU:HD22	1:A:317:PRO:HB2	1.97	0.46
1:E:318:THR:HG21	1:E:353:GLU:HB3	1.97	0.46
2:B:627:LEU:HD13	2:B:640:VAL:HG13	1.97	0.46
2:B:619:GLU:OE2	2:B:650:ARG:HD3	2.15	0.46
1:C:215:TYR:CD2	1:C:397:MET:HE1	2.51	0.46
2:D:608:ASN:HD22	2:D:608:ASN:N	2.14	0.46
2:B:560:GLU:OE1	6:B:773:HOH:O	2.21	0.46
1:C:247:HIS:HD2	6:C:1805:HOH:O	1.99	0.46
1:C:107:ARG:HH22	5:C:1701:MPD:H31	1.80	0.46
1:C:116:SER:OG	1:C:118:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:THR:CG2	6:E:1720:HOH:O	2.61	0.46
2:B:546:THR:HG23	2:B:548:ASP:H	1.80	0.46
1:E:327:HIS:HE1	6:E:1841:HOH:O	1.99	0.45
1:A:17:VAL:O	1:A:425:ARG:HD2	2.16	0.45
1:A:61:TYR:CE1	1:A:96:CYS:SG	3.10	0.45
1:C:245:THR:HG22	1:C:246:GLY:O	2.16	0.45
2:F:546:THR:CG2	2:F:548:ASP:OD1	2.64	0.45
1:E:215:TYR:CG	1:E:397:MET:HE1	2.51	0.45
1:E:383:MET:HE3	1:E:383:MET:HA	1.99	0.45
1:C:198:VAL:HG11	1:C:333:LYS:HE3	1.99	0.45
2:D:622:VAL:HG21	2:D:649:LEU:HD22	1.98	0.45
1:E:309:MET:HB2	1:E:309:MET:HE2	1.75	0.44
2:B:572:THR:HG23	2:B:574:MET:N	2.32	0.44
2:D:557:VAL:O	2:D:566:ASP:HB2	2.17	0.44
2:F:546:THR:CG2	2:F:659:ALA:HA	2.47	0.44
2:D:546:THR:HG21	2:D:659:ALA:HA	1.99	0.44
1:E:25:ALA:HB1	1:E:383:MET:HE1	2.00	0.44
1:E:198:VAL:HG11	1:E:333:LYS:HE3	2.00	0.44
1:E:440:PRO:O	1:E:441:LEU:HB2	2.18	0.44
1:A:318:THR:HG21	1:A:353:GLU:HB3	2.00	0.43
1:C:25:ALA:HB1	1:C:383:MET:HE1	1.98	0.43
1:E:136:LYS:HE2	6:E:1910:HOH:O	2.19	0.43
1:E:128:LYS:CD	1:E:129:ASP:N	2.75	0.43
1:E:341:LEU:HD12	1:E:341:LEU:N	2.34	0.43
1:A:25:ALA:HB1	1:A:383:MET:HE2	2.00	0.43
1:A:116:SER:OG	1:A:118:THR:HB	2.19	0.43
1:A:440:PRO:O	1:A:441:LEU:HB2	2.18	0.43
2:F:602:SER:HA	2:F:629:TYR:O	2.19	0.42
1:A:245:THR:HG22	1:A:246:GLY:O	2.19	0.42
1:A:56:PRO:HD2	1:A:60:ASP:OD2	2.20	0.42
1:C:151:TYR:CE2	1:C:174:LYS:HD2	2.55	0.41
1:C:289:ARG:HB3	1:C:290:PRO:HD3	2.02	0.41
1:C:385:GLY:HA3	1:E:69:ASP:OD1	2.20	0.41
1:C:398:GLY:HA3	1:C:402:LEU:HG	2.02	0.41
1:C:93:MET:HG2	1:C:94:GLN:N	2.36	0.41
1:C:440:PRO:O	1:C:441:LEU:HB2	2.21	0.41
1:A:355:TYR:OH	2:B:572:THR:HB	2.21	0.41
1:A:289:ARG:HB3	1:A:290:PRO:HD3	2.02	0.41
1:C:193:ALA:HB1	1:C:194:PRO:HD2	2.03	0.41
1:A:200:ASP:OD1	1:A:200:ASP:N	2.51	0.41
1:E:382:VAL:HG22	6:E:1745:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:THR:CG2	2:B:548:ASP:OD1	2.69	0.40
2:B:557:VAL:O	2:B:566:ASP:HB2	2.21	0.40
1:A:128:LYS:HD2	1:A:129:ASP:N	2.26	0.40
5:E:1711:MPD:HM3	5:E:1711:MPD:O4	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	439/470 (93%)	425 (97%)	12 (3%)	2 (0%)	24	21
1	C	439/470 (93%)	423 (96%)	15 (3%)	1 (0%)	43	42
1	E	439/470 (93%)	428 (98%)	9 (2%)	2 (0%)	24	21
2	B	165/172 (96%)	155 (94%)	7 (4%)	3 (2%)	6	3
2	D	165/172 (96%)	156 (94%)	6 (4%)	3 (2%)	6	3
2	F	165/172 (96%)	155 (94%)	7 (4%)	3 (2%)	6	3
All	All	1812/1926 (94%)	1742 (96%)	56 (3%)	14 (1%)	16	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	514	VAL
2	B	516	ASP
2	D	514	VAL
2	D	516	ASP
2	F	514	VAL
2	F	516	ASP
1	E	440	PRO
2	B	515	SER

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Mol	Chain	Res	Type
1	C	440	PRO
2	D	515	SER
2	F	515	SER
1	A	440	PRO
1	E	212	GLY
1	A	212	GLY

5.3.2 Protein sidechains ⓘ

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	371/389 (95%)	352 (95%)	19 (5%)	21	19
1	C	371/389 (95%)	353 (95%)	18 (5%)	22	20
1	E	371/389 (95%)	350 (94%)	21 (6%)	18	15
2	B	147/154 (96%)	137 (93%)	10 (7%)	14	11
2	D	147/154 (96%)	136 (92%)	11 (8%)	12	9
2	F	147/154 (96%)	135 (92%)	12 (8%)	10	7
All	All	1554/1629 (95%)	1463 (94%)	91 (6%)	18	14

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	41	ILE
1	A	107	ARG
1	A	118	THR
1	A	128	LYS
1	A	150	SER
1	A	159	LEU
1	A	166	LEU
1	A	173	LEU
1	A	180	VAL
1	A	188	LEU
1	A	229	LEU

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Mol	Chain	Res	Type
1	A	245	THR
1	A	260	MET
1	A	278	ARG
1	A	308	LEU
1	A	309	MET
1	A	318	THR
1	A	441	LEU
2	B	517	THR
2	B	533	LEU
2	B	546	THR
2	B	552	VAL
2	B	572	THR
2	B	617	GLU
2	B	618	ASP
2	B	627	LEU
2	B	649	LEU
2	B	657	LEU
1	C	1	MET
1	C	107	ARG
1	C	118	THR
1	C	128	LYS
1	C	150	SER
1	C	159	LEU
1	C	166	LEU
1	C	173	LEU
1	C	180	VAL
1	C	188	LEU
1	C	229	LEU
1	C	245	THR
1	C	260	MET
1	C	278	ARG
1	C	308	LEU
1	C	309	MET
1	C	318	THR
1	C	441	LEU
2	D	517	THR
2	D	533	LEU
2	D	546	THR
2	D	552	VAL
2	D	572	THR
2	D	608	ASN
2	D	617	GLU

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Mol	Chain	Res	Type
2	D	618	ASP
2	D	627	LEU
2	D	649	LEU
2	D	657	LEU
1	E	1	MET
1	E	41	ILE
1	E	107	ARG
1	E	118	THR
1	E	128	LYS
1	E	150	SER
1	E	154	LEU
1	E	159	LEU
1	E	166	LEU
1	E	173	LEU
1	E	180	VAL
1	E	188	LEU
1	E	229	LEU
1	E	245	THR
1	E	260	MET
1	E	276	LEU
1	E	278	ARG
1	E	308	LEU
1	E	309	MET
1	E	318	THR
1	E	441	LEU
2	F	517	THR
2	F	533	LEU
2	F	546	THR
2	F	552	VAL
2	F	572	THR
2	F	608	ASN
2	F	616	SER
2	F	617	GLU
2	F	618	ASP
2	F	627	LEU
2	F	649	LEU
2	F	657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	327	HIS
2	B	608	ASN
1	C	327	HIS
2	D	608	ASN
1	E	133	ASN
1	E	247	HIS
1	E	327	HIS
1	E	396	GLN
2	F	608	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	MPD	E	1713	-	7,7,7	0.39	0	9,10,10	0.90	0
5	MPD	A	1702	-	7,7,7	0.35	0	9,10,10	0.34	0
5	MPD	C	1701	-	7,7,7	0.29	0	9,10,10	0.47	0
4	FES	C	501	1	0,4,4	-	-	-	-	-
5	MPD	C	1704	-	7,7,7	0.45	0	9,10,10	0.96	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	E	1708	-	7,7,7	0.40	0	9,10,10	0.59	0
5	MPD	E	1711	-	7,7,7	0.63	0	9,10,10	0.24	0
4	FES	A	501	1	0,4,4	-	-	-		
5	MPD	C	1707	-	7,7,7	0.82	0	9,10,10	0.86	1 (11%)
5	MPD	E	1710	-	7,7,7	0.28	0	9,10,10	0.36	0
4	FES	E	501	1	0,4,4	-	-	-		
5	MPD	A	1703	-	7,7,7	0.62	0	9,10,10	0.50	0
5	MPD	A	1709	-	7,7,7	0.32	0	9,10,10	0.33	0
5	MPD	A	1700	-	7,7,7	0.57	0	9,10,10	0.82	0
5	MPD	E	1712	-	7,7,7	0.23	0	9,10,10	0.68	0
5	MPD	E	1705	-	7,7,7	0.42	0	9,10,10	0.36	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	MPD	E	1713	-	-	2/5/5/5	-
5	MPD	A	1702	-	-	1/5/5/5	-
5	MPD	C	1701	-	-	1/5/5/5	-
5	MPD	E	1708	-	-	0/5/5/5	-
5	MPD	C	1704	-	-	1/5/5/5	-
5	MPD	E	1711	-	-	1/5/5/5	-
4	FES	C	501	1	-	-	0/1/1/1
4	FES	A	501	1	-	-	0/1/1/1
5	MPD	C	1707	-	-	0/5/5/5	-
5	MPD	E	1710	-	-	0/5/5/5	-
4	FES	E	501	1	-	-	0/1/1/1
5	MPD	A	1709	-	-	2/5/5/5	-
5	MPD	A	1703	-	-	1/5/5/5	-
5	MPD	A	1700	-	-	0/5/5/5	-
5	MPD	E	1712	-	-	1/5/5/5	-
5	MPD	E	1705	-	-	3/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1704	MPD	CM-C2-C1	-2.49	105.06	110.63
5	C	1707	MPD	CM-C2-C1	-2.04	106.05	110.63

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1709	MPD	C2-C3-C4-O4
5	C	1701	MPD	C2-C3-C4-C5
5	E	1705	MPD	C2-C3-C4-O4
5	E	1713	MPD	C2-C3-C4-O4
5	E	1713	MPD	C2-C3-C4-C5
5	E	1711	MPD	O2-C2-C3-C4
5	A	1702	MPD	C2-C3-C4-C5
5	A	1709	MPD	C2-C3-C4-C5
5	E	1705	MPD	C2-C3-C4-C5
5	E	1712	MPD	C2-C3-C4-C5
5	A	1703	MPD	O2-C2-C3-C4
5	C	1704	MPD	O2-C2-C3-C4
5	E	1705	MPD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1701	MPD	2	0
5	E	1711	MPD	1	0
5	C	1707	MPD	3	0
5	E	1712	MPD	2	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 ⓘ

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, 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	441/470 (93%)	0.08	3 (0%) 84 84	9, 15, 27, 60	0
1	C	441/470 (93%)	0.09	13 (2%) 53 52	9, 15, 27, 60	0
1	E	441/470 (93%)	-0.10	7 (1%) 70 70	9, 15, 27, 60	0
2	B	167/172 (97%)	-0.01	4 (2%) 59 59	10, 17, 38, 63	0
2	D	167/172 (97%)	-0.02	7 (4%) 40 39	10, 17, 38, 63	0
2	F	167/172 (97%)	-0.03	5 (2%) 52 51	10, 17, 38, 63	0
All	All	1824/1926 (94%)	0.01	39 (2%) 63 63	9, 15, 32, 63	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	441	LEU	6.5
1	A	441	LEU	5.8
1	E	440	PRO	5.6
1	E	441	LEU	4.5
2	B	515	SER	4.0
1	E	439	SER	3.9
2	F	515	SER	3.8
2	F	516	ASP	3.8
2	D	515	SER	3.7
2	F	514	VAL	3.7
2	B	514	VAL	3.4
2	D	617	GLU	3.3
1	A	259	GLY	3.1
1	E	1	MET	3.1
1	C	261	PRO	3.0
2	D	514	VAL	3.0
1	C	128	LYS	3.0
2	D	618	ASP	3.0
1	C	259	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.8
1	C	439	SER	2.8
1	A	258	PRO	2.8
2	D	654	ASP	2.7
2	F	617	GLU	2.6
1	C	260	MET	2.6
2	D	517	THR	2.5
1	C	440	PRO	2.5
2	F	513	ARG	2.5
1	C	400	GLY	2.4
1	C	124	VAL	2.4
1	E	258	PRO	2.3
2	D	516	ASP	2.3
2	B	513	ARG	2.3
1	C	270	GLU	2.3
1	C	109	PRO	2.2
1	C	2	LEU	2.0
2	B	516	ASP	2.0
1	E	260	MET	2.0
1	E	259	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	MPD	E	1713	8/8	0.61	0.17	41,44,44,44	0
5	MPD	A	1709	8/8	0.66	0.21	71,72,73,73	0
5	MPD	A	1702	8/8	0.66	0.19	68,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	A	1703	8/8	0.74	0.19	30,33,36,38	0
5	MPD	E	1712	8/8	0.75	0.21	63,64,65,65	0
5	MPD	E	1710	8/8	0.75	0.24	97,97,97,97	0
5	MPD	E	1705	8/8	0.77	0.18	56,59,61,61	0
5	MPD	C	1701	8/8	0.78	0.23	75,76,79,79	0
5	MPD	E	1711	8/8	0.80	0.15	33,34,35,36	0
5	MPD	C	1707	8/8	0.83	0.12	20,24,28,28	0
5	MPD	A	1700	8/8	0.88	0.09	25,28,32,33	0
5	MPD	C	1704	8/8	0.89	0.11	26,29,34,34	0
5	MPD	E	1708	8/8	0.92	0.08	24,30,34,39	0
3	FE	C	502	1/1	0.99	0.01	21,21,21,21	0
3	FE	E	502	1/1	0.99	0.02	21,21,21,21	0
4	FES	A	501	4/4	0.99	0.04	20,20,20,22	0
4	FES	C	501	4/4	0.99	0.03	20,20,21,21	0
4	FES	E	501	4/4	0.99	0.04	19,19,19,20	0
3	FE	A	502	1/1	0.99	0.02	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.