



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:55 PM GMT

PDB ID : 1D2V
Title : CRYSTAL STRUCTURE OF BROMIDE-BOUND HUMAN MYELOPER-
OXIDASE ISOFORM C AT PH 5.5
Authors : Fiedler, T.J.; Davey, C.A.; Fenna, R.E.
Deposited on : 1999-09-28
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

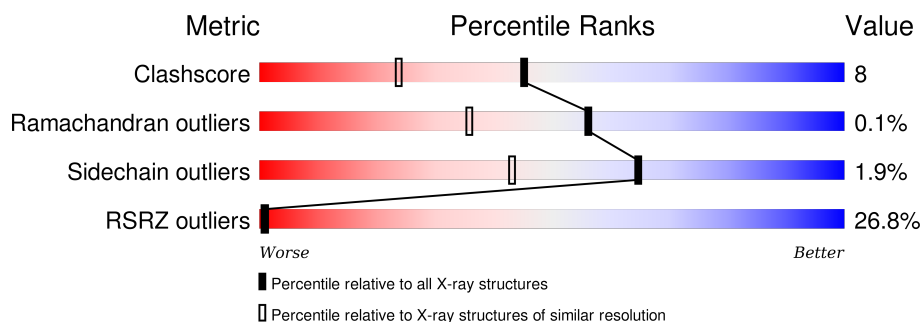
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	104	
1	B	104	
2	C	466	
2	D	466	

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	BMA	C	1642	-	-	-	X
6	BR	A	843	-	-	X	-
8	ACT	C	1606	-	-	X	X
8	ACT	D	2604	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10306 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			
2	D	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164
D	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	6	Total	C	N	O	0	0
			71	40	2	29		
3	D	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is BROMIDE ION (three-letter code: BR) (formula: Br).

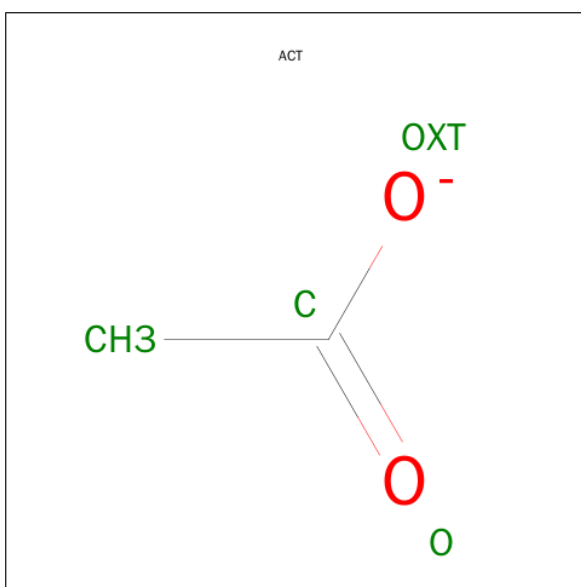
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Br	0	0
			4	4		
6	A	4	Total	Br	0	0
			4	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



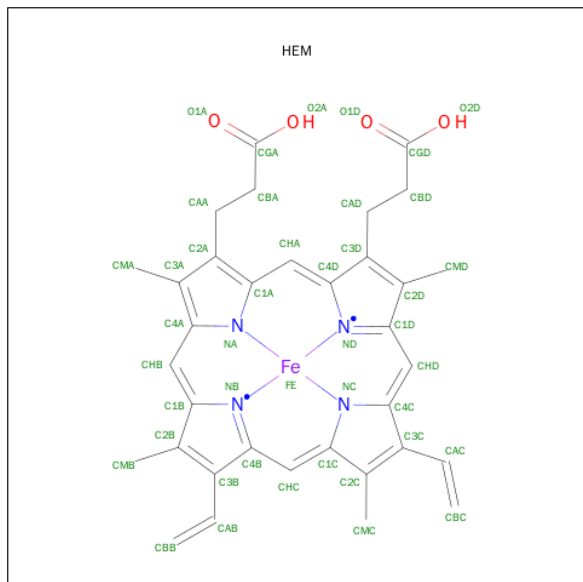
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



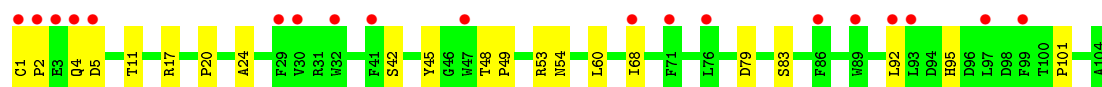
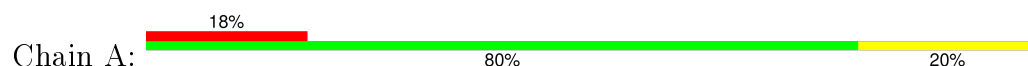
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	319	Total 319	O 319	0	0
10	D	314	Total 314	O 314	0	0

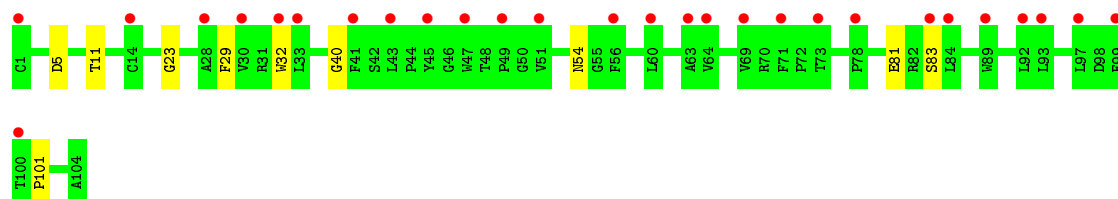
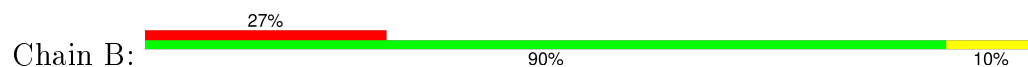
3 Residue-property plots [i](#)

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

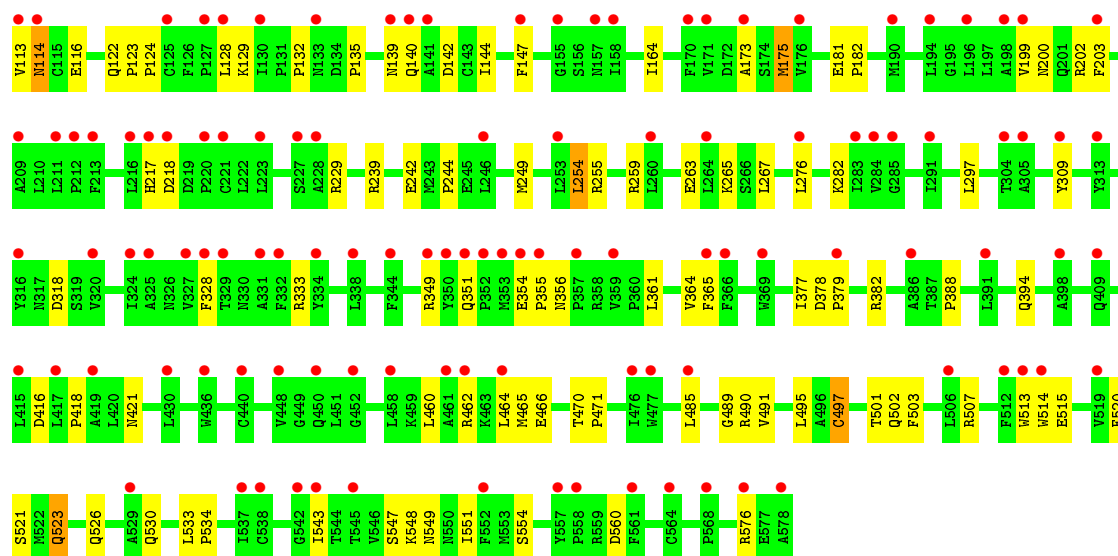
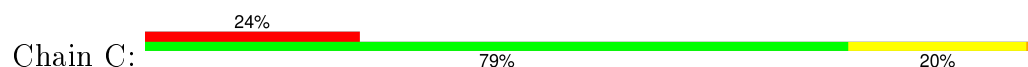
- Molecule 1: MYELOPEROXIDASE



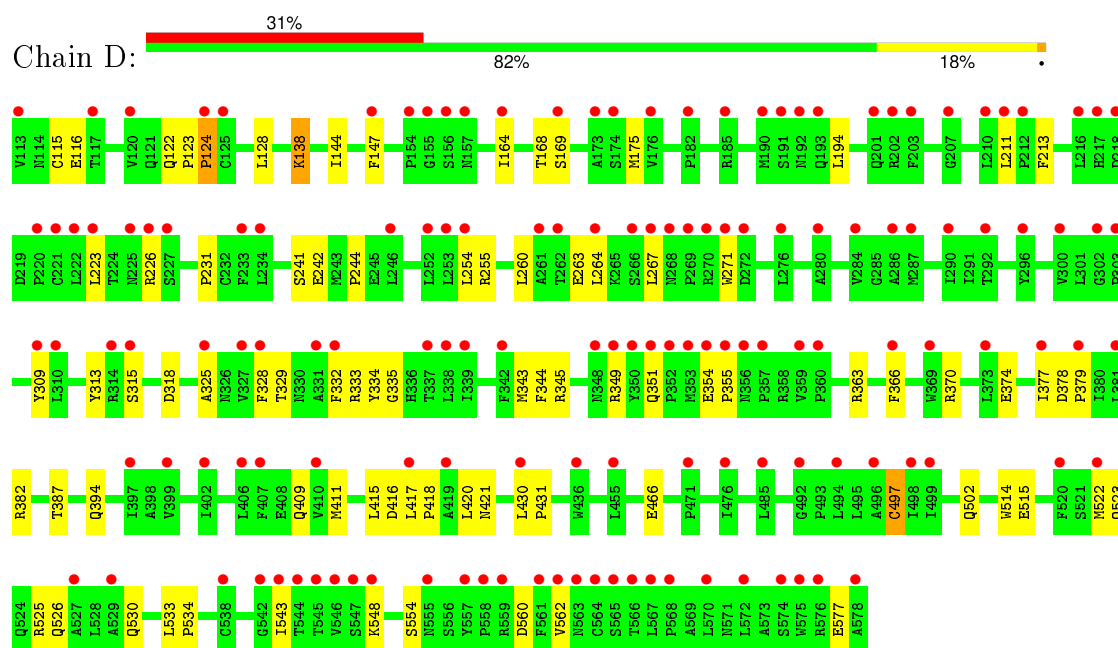
- Molecule 1: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



- Molecule 2: MYELOPEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.16 Å 63.49 Å 92.48 Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 44.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-1.75) 90.4 (44.41-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.76 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.243 , 0.296 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 115555 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, BMA, NAG, CA, FUC, BR, ACT, HEM, MAN, SO4

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	0.75	0/863	0.73	0/1174
1	B	0.76	0/863	0.72	0/1174
2	C	0.73	1/3811 (0.0%)	0.65	0/5168
2	D	0.70	0/3811	0.63	0/5168
All	All	0.72	1/9348 (0.0%)	0.66	0/12684

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	114	ASN	C-N	-6.21	1.19	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	838	0	798	17	0
1	B	838	0	798	8	0
2	C	3733	0	3723	65	0
2	D	3733	0	3725	65	0
3	C	71	0	61	0	0
3	D	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	26	1	0
4	D	28	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	3	0
6	B	4	0	0	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	C	12	0	9	4	0
8	D	12	0	9	3	0
9	A	43	0	30	3	0
9	B	43	0	30	2	0
10	A	98	0	0	4	0
10	B	100	0	0	1	0
10	C	319	0	0	10	0
10	D	314	0	0	4	0
All	All	10306	0	9296	147	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 8.

All (147) 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:C:355:PRO:HG2	2:C:356:ASN:HD22	1.44	0.82
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.31	0.78
2:C:132:PRO:HG3	2:C:140:GLN:NE2	2.04	0.72
2:C:355:PRO:HG2	2:C:356:ASN:ND2	2.05	0.71
2:C:200:ASN:HD22	2:C:203:PHE:H	1.36	0.70
2:C:123:PRO:HB3	8:C:1606:ACT:H3	1.74	0.69
2:D:122:GLN:HA	2:D:122:GLN:HE21	1.55	0.69
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.73	0.69
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.76	0.69
4:C:1620:NAG:H5	10:C:1250(A):HOH:O	1.92	0.68
2:D:211:LEU:HD23	2:D:254:LEU:HD22	1.76	0.66
2:D:333:ARG:HH11	2:D:421:ASN:ND2	1.94	0.65
10:A:1243(A):HOH:O	2:C:129:LYS:HD3	1.98	0.64
2:D:128:LEU:HB2	2:D:144:ILE:HB	1.80	0.64
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.80	0.63
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASP:HB3	10:B:1272(B):HOH:O	1.99	0.62
2:D:548:LYS:HE2	2:D:562:VAL:HG13	1.83	0.61
9:A:605:HEM:HBB2	2:C:242:GLU:OE1	2.00	0.61
2:C:200:ASN:ND2	2:C:203:PHE:H	1.98	0.60
2:D:122:GLN:HA	2:D:122:GLN:NE2	2.17	0.59
6:A:843:BR:BR	2:C:242:GLU:HG3	2.57	0.59
2:D:263:GLU:HG3	10:D:921(B):HOH:O	2.02	0.58
2:D:522:MET:HG3	8:D:2604:ACT:H1	1.84	0.58
1:A:2:PRO:HD2	10:A:791(A):HOH:O	2.04	0.58
2:D:122:GLN:HE21	2:D:123:PRO:CD	2.15	0.58
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.52	0.57
2:D:122:GLN:HE21	2:D:123:PRO:HD3	1.71	0.56
2:C:135:PRO:HG2	10:C:1204(A):HOH:O	2.05	0.56
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.88	0.56
6:A:843:BR:BR	10:C:957(A):HOH:O	2.73	0.56
1:A:101:PRO:HB2	10:A:1247(A):HOH:O	2.05	0.55
2:C:382:ARG:NH1	10:C:777(A):HOH:O	2.37	0.54
1:A:83:SER:HB3	2:C:554:SER:O	2.08	0.54
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.88	0.53
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.91	0.53
2:D:378:ASP:HB2	2:D:379:PRO:HD3	1.91	0.53
2:D:548:LYS:HE2	2:D:562:VAL:CG1	2.38	0.53
2:D:271:TRP:HE1	2:D:577:GLU:CD	2.12	0.52
2:D:382:ARG:HG3	2:D:543:ILE:CD1	2.39	0.52
2:D:411:MET:CE	2:D:415:LEU:HD21	2.40	0.51
2:D:138:LYS:HZ3	2:D:138:LYS:HA	1.76	0.51
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.51
1:B:83:SER:HB3	2:D:554:SER:O	2.10	0.51
2:C:113:VAL:HG12	2:C:114:ASN:N	2.26	0.51
2:C:521:SER:OG	2:C:523:GLN:HG2	2.10	0.51
2:C:507:ARG:HG3	2:C:513:TRP:CE2	2.46	0.51
2:C:114:ASN:HA	10:C:973(A):HOH:O	2.11	0.51
2:D:255:ARG:NH1	2:D:377:ILE:HD11	2.26	0.51
2:D:138:LYS:NZ	2:D:138:LYS:HA	2.25	0.50
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.11	0.50
2:D:328:PHE:CD1	2:D:502:GLN:HG2	2.46	0.50
2:D:244:PRO:HB2	2:D:343:MET:SD	2.51	0.50
2:D:116:GLU:OE1	2:D:411:MET:HE3	2.11	0.49
9:A:605:HEM:HMC2	9:A:605:HEM:HBC2	1.94	0.49
2:C:465:MET:CE	2:C:471:PRO:HD3	2.42	0.49
2:C:394:GLN:HB3	2:C:460:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:ASP:O	2:D:420:LEU:HG	2.11	0.49
2:C:548:LYS:HD2	2:C:560:ASP:HA	1.94	0.49
1:A:20:PRO:HG2	1:B:40:GLY:HA3	1.95	0.48
1:A:92:LEU:HD22	2:C:249:MET:HB3	1.96	0.48
2:D:416:ASP:OD2	2:D:418:PRO:HD2	2.13	0.48
1:A:17:ARG:HB3	10:A:915(B):HOH:O	2.13	0.48
2:C:549:ASN:HB3	10:C:1232(A):HOH:O	2.13	0.48
2:C:549:ASN:ND2	10:C:829(A):HOH:O	2.46	0.47
2:C:116:GLU:HG3	2:C:147:PHE:CZ	2.48	0.47
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.49	0.47
2:D:554:SER:HB3	2:D:560:ASP:HB3	1.95	0.47
2:D:213:PHE:CD2	2:D:231:PRO:HG2	2.50	0.47
2:C:173:ALA:HA	2:C:175:MET:SD	2.55	0.47
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.96	0.47
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.97	0.47
2:C:123:PRO:CB	8:C:1606:ACT:H3	2.42	0.46
2:D:394:GLN:HG3	10:D:850(B):HOH:O	2.15	0.46
2:D:378:ASP:O	2:D:543:ILE:HD11	2.15	0.46
2:C:462:ARG:O	2:C:466:GLU:HG2	2.15	0.46
2:D:345:ARG:NH1	10:D:762(B):HOH:O	2.48	0.46
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.30	0.46
6:A:758:BR:BR	2:C:543:ILE:HG23	2.70	0.46
2:C:361:LEU:O	2:C:364:VAL:HG22	2.16	0.46
2:D:533:LEU:HB3	2:D:534:PRO:HD3	1.98	0.46
2:C:297:LEU:HD11	2:C:503:PHE:CD1	2.51	0.46
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.51	0.46
2:C:200:ASN:ND2	2:C:202:ARG:H	2.14	0.45
1:A:1:CYS:SG	1:A:20:PRO:HB3	2.56	0.45
2:C:181:GLU:HB2	2:C:182:PRO:HD3	1.98	0.45
2:D:260:LEU:O	2:D:264:LEU:HG	2.17	0.45
2:C:416:ASP:OD2	2:C:418:PRO:HD2	2.15	0.45
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.51	0.45
2:C:255:ARG:NH1	2:C:377:ILE:HD11	2.32	0.45
2:D:122:GLN:HE21	2:D:122:GLN:CA	2.25	0.45
2:D:123:PRO:HA	2:D:124:PRO:HA	1.83	0.45
2:D:223:LEU:HD22	2:D:226:ARG:NH1	2.31	0.45
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.99	0.45
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.99	0.45
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.98	0.44
9:A:605:HEM:HBC2	9:A:605:HEM:CMC	2.46	0.44
2:C:135:PRO:CG	10:C:1204(A):HOH:O	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE1	1:A:53:ARG:HG3	2.53	0.44
2:D:241:SER:O	2:D:366:PHE:HA	2.18	0.44
2:C:378:ASP:HB2	2:C:379:PRO:HD3	2.00	0.44
2:C:259:ARG:O	2:C:263:GLU:HG3	2.17	0.44
2:C:513:TRP:CD1	2:C:515:GLU:HB2	2.53	0.43
2:D:533:LEU:N	2:D:534:PRO:CD	2.81	0.43
6:B:843:BR:BR	2:D:242:GLU:HG3	2.74	0.43
2:C:229:ARG:HG2	2:C:229:ARG:HH11	1.84	0.43
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.43
1:A:68:ILE:HD13	2:C:464:LEU:HD23	2.00	0.43
1:A:101:PRO:HD2	2:C:164:ILE:O	2.18	0.43
2:D:194:LEU:HD13	10:D:948(B):HOH:O	2.18	0.43
1:A:79:ASP:O	2:C:388:PRO:HB3	2.19	0.43
2:D:526:GLN:NE2	2:D:530:GLN:HE21	2.17	0.43
2:C:124:PRO:HA	8:C:1606:ACT:H1	2.00	0.43
2:C:244:PRO:HD3	2:C:364:VAL:O	2.18	0.43
9:B:605:HEM:CBC	2:D:335:GLY:HA3	2.48	0.43
1:B:23:GLY:HA2	2:D:169:SER:OG	2.19	0.42
2:C:533:LEU:HB3	2:C:534:PRO:HD3	2.01	0.42
2:C:501:THR:HA	10:C:814(A):HOH:O	2.19	0.42
1:A:45:TYR:CZ	1:A:53:ARG:HG3	2.55	0.42
2:D:344:PHE:CD1	2:D:387:THR:HG21	2.55	0.42
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.54	0.42
2:C:242:GLU:O	2:C:365:PHE:HA	2.20	0.42
2:D:313:TYR:CZ	2:D:315:SER:HA	2.54	0.42
2:C:526:GLN:NE2	2:C:530:GLN:NE2	2.68	0.42
2:D:116:GLU:OE2	2:D:411:MET:HB2	2.20	0.42
9:B:605:HEM:HBB2	2:D:242:GLU:OE1	2.20	0.42
8:C:1606:ACT:H2	10:C:1213(A):HOH:O	2.19	0.41
2:D:332:PHE:C	2:D:334:TYR:H	2.24	0.41
1:B:11:THR:O	2:D:168:THR:HG22	2.20	0.41
1:A:4:GLN:HG2	1:A:5:ASP:N	2.35	0.41
2:D:430:LEU:HA	2:D:431:PRO:HD3	1.97	0.41
2:C:547:SER:HB2	2:C:551:ILE:HG13	2.03	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:11:THR:O	1:A:24:ALA:HA	2.20	0.41
1:B:29:PHE:CZ	2:D:329:THR:HG21	2.56	0.41
2:D:309:TYR:CZ	2:D:497:CYS:HA	2.55	0.41
2:D:525:ARG:HH21	8:D:2604:ACT:CH3	2.33	0.41
1:A:60:LEU:HD12	1:A:60:LEU:N	2.36	0.41
1:A:95:HIS:CD2	2:C:239:ARG:CZ	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:LEU:HD12	2:C:576:ARG:HB2	2.03	0.40
2:C:309:TYR:CZ	2:C:497:CYS:HA	2.56	0.40
2:C:328:PHE:CD1	2:C:502:GLN:HG2	2.56	0.40
2:C:489:GLY:O	2:C:490:ARG:HD3	2.21	0.40
2:D:363:ARG:HG2	2:D:409:GLN:NE2	2.36	0.40
2:D:525:ARG:HH21	8:D:2604:ACT:C	2.34	0.40
2:D:370:ARG:O	2:D:374:GLU:HB2	2.21	0.40
2:D:466:GLU:HG2	2:D:466:GLU:O	2.22	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	102/104 (98%)	100 (98%)	1 (1%)	1 (1%)	19	5
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	C	463/466 (99%)	445 (96%)	18 (4%)	0	100	100
2	D	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
All	All	1130/1140 (99%)	1094 (97%)	35 (3%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER

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	90/90 (100%)	89 (99%)	1 (1%)	80	66
1	B	90/90 (100%)	88 (98%)	2 (2%)	60	35
2	C	410/410 (100%)	401 (98%)	9 (2%)	60	35
2	D	410/410 (100%)	403 (98%)	7 (2%)	68	49
All	All	1000/1000 (100%)	981 (98%)	19 (2%)	65	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	122	GLN
2	C	175	MET
2	C	217	HIS
2	C	218	ASP
2	C	254	LEU
2	C	318	ASP
2	C	470	THR
2	C	497	CYS
2	C	523	GLN
1	B	54	ASN
1	B	81	GLU
2	D	124	PRO
2	D	138	LYS
2	D	175	MET
2	D	267	LEU
2	D	318	ASP
2	D	497	CYS
2	D	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	140	GLN
2	C	200	ASN
2	C	201	GLN
2	C	356	ASN
2	C	526	GLN

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Mol	Chain	Res	Type
2	C	530	GLN
2	C	549	ASN
1	B	54	ASN
2	D	122	GLN
2	D	421	ASN
2	D	526	GLN
2	D	549	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	$\# Z > 2$
2	CSO	C	150	2	3,6,7	0.66	0	1,6,8	1.98	0
2	CSO	D	150	2	3,6,7	0.82	0	1,6,8	1.94	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
2	CSO	C	150	2	-	0/1/5/7	0/0/0/0
2	CSO	D	150	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

12 carbohydrates 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	$\# Z > 2$
3	NAG	C	1640	3,2	14,14,15	0.84	0	15,19,21	0.94	1 (6%)
3	NAG	C	1641	3	14,14,15	0.74	0	15,19,21	0.81	0
3	BMA	C	1642	3	11,11,12	0.69	0	14,15,17	0.62	0
3	MAN	C	1643	3	11,11,12	0.65	0	14,15,17	0.87	1 (7%)
3	MAN	C	1644	3	11,11,12	0.54	0	14,15,17	0.76	0
3	FUC	C	1645	3	10,10,11	0.64	0	14,14,16	0.71	0
3	NAG	D	2640	3,2	14,14,15	0.69	0	15,19,21	1.23	1 (6%)
3	NAG	D	2641	3	14,14,15	0.85	0	15,19,21	0.99	1 (6%)
3	BMA	D	2642	3	11,11,12	0.86	1 (9%)	14,15,17	0.65	0
3	MAN	D	2643	3	11,11,12	0.77	0	14,15,17	1.06	1 (7%)
3	MAN	D	2644	3	11,11,12	0.73	0	14,15,17	0.69	0
3	FUC	D	2645	3	10,10,11	0.91	0	14,14,16	0.71	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
3	NAG	C	1640	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	1641	3	-	0/6/23/26	0/1/1/1
3	BMA	C	1642	3	-	0/2/19/22	0/1/1/1
3	MAN	C	1643	3	-	0/2/19/22	0/1/1/1
3	MAN	C	1644	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	C	1645	3	-	0/0/17/20	0/1/1/1
3	NAG	D	2640	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	2641	3	-	0/6/23/26	0/1/1/1
3	BMA	D	2642	3	-	0/2/19/22	0/1/1/1
3	MAN	D	2643	3	-	0/2/19/22	0/1/1/1
3	MAN	D	2644	3	-	0/2/19/22	0/1/1/1
3	FUC	D	2645	3	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2642	BMA	C2-C3	2.04	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2640	NAG	C2-N2-C7	-3.55	118.48	123.04
3	D	2641	NAG	C2-N2-C7	-3.07	119.09	123.04
3	C	1640	NAG	C2-N2-C7	-2.19	120.22	123.04
3	C	1643	MAN	C1-O5-C5	2.05	114.85	112.25
3	D	2643	MAN	C1-O5-C5	3.18	116.28	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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
7	SO4	A	1602	-	4,4,4	0.11	0	6,6,6	0.24	0
9	HEM	A	605	1,10,2	30,50,50	2.73	8 (26%)	24,82,82	2.05	6 (25%)
7	SO4	B	2602	-	4,4,4	0.25	0	6,6,6	0.09	0
9	HEM	B	605	1,10,2	30,50,50	2.41	9 (30%)	24,82,82	2.02	6 (25%)
7	SO4	C	1603	-	4,4,4	0.22	0	6,6,6	0.09	0
8	ACT	C	1604	-	1,3,3	3.14	1 (100%)	0,3,3	0.00	-
8	ACT	C	1606	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
8	ACT	C	1607	-	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
4	NAG	C	1620	2	14,14,15	0.64	0	15,19,21	1.14	1 (6%)
4	NAG	C	1630	2	14,14,15	0.52	0	15,19,21	0.90	1 (6%)
8	ACT	D	2604	-	1,3,3	3.09	1 (100%)	0,3,3	0.00	-
8	ACT	D	2606	-	1,3,3	2.05	1 (100%)	0,3,3	0.00	-
8	ACT	D	2607	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
4	NAG	D	2620	2	14,14,15	0.53	0	15,19,21	0.80	0
4	NAG	D	2630	2	14,14,15	0.78	0	15,19,21	0.95	1 (6%)

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
7	SO4	A	1602	-	-	0/0/0/0	0/0/0/0
9	HEM	A	605	1,10,2	-	0/10/54/54	0/0/8/8
7	SO4	B	2602	-	-	0/0/0/0	0/0/0/0
9	HEM	B	605	1,10,2	-	0/10/54/54	0/0/8/8
7	SO4	C	1603	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1604	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1606	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1607	-	-	0/0/0/0	0/0/0/0
4	NAG	C	1620	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
8	ACT	D	2604	-	-	0/0/0/0	0/0/0/0
8	ACT	D	2606	-	-	0/0/0/0	0/0/0/0
8	ACT	D	2607	-	-	0/0/0/0	0/0/0/0
4	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
4	NAG	D	2630	2	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	605	HEM	C3C-CAC	-6.39	1.39	1.51
9	A	605	HEM	C3B-C4B	-5.95	1.46	1.51
9	A	605	HEM	C3B-CAB	-5.85	1.40	1.51
9	A	605	HEM	C2D-C3D	-5.85	1.37	1.54
9	B	605	HEM	C2D-C3D	-5.70	1.37	1.54
9	A	605	HEM	C3D-C4D	-5.20	1.44	1.51
9	B	605	HEM	C3B-CAB	-5.09	1.41	1.51
9	B	605	HEM	C2C-C1C	-4.80	1.43	1.52
9	B	605	HEM	C3B-C4B	-4.63	1.47	1.51
9	B	605	HEM	C3C-CAC	-4.58	1.42	1.51
9	B	605	HEM	C3D-C4D	-3.99	1.46	1.51
9	A	605	HEM	C2C-C1C	-3.83	1.45	1.52
8	D	2606	ACT	CH3-C	2.05	1.51	1.48
8	C	1606	ACT	CH3-C	2.44	1.52	1.48
9	B	605	HEM	C1C-NC	2.48	1.39	1.36
9	A	605	HEM	CBC-CAC	2.53	1.43	1.29
9	A	605	HEM	CBB-CAB	2.83	1.45	1.29
9	B	605	HEM	CBC-CAC	2.88	1.46	1.29
9	B	605	HEM	CBB-CAB	2.93	1.46	1.29
8	D	2604	ACT	CH3-C	3.09	1.53	1.48
8	D	2607	ACT	CH3-C	3.13	1.53	1.48
8	C	1604	ACT	CH3-C	3.14	1.53	1.48
8	C	1607	ACT	CH3-C	3.54	1.53	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1620	NAG	C2-N2-C7	-2.84	119.39	123.04
4	D	2630	NAG	C1-O5-C5	-2.48	109.10	112.25
4	C	1630	NAG	C2-N2-C7	-2.17	120.25	123.04
9	B	605	HEM	C2D-C3D-C4D	2.35	105.49	101.50
9	A	605	HEM	C2D-C3D-C4D	2.41	105.59	101.50
9	B	605	HEM	CMD-C2D-C3D	2.95	127.38	114.35
9	A	605	HEM	CMD-C2D-C3D	3.02	127.70	114.35
9	B	605	HEM	CAD-C3D-C4D	3.64	125.33	112.47
9	A	605	HEM	CAD-C3D-C4D	3.81	125.91	112.47
9	B	605	HEM	CMB-C2B-C3B	3.88	126.21	116.53
9	A	605	HEM	CMB-C2B-C3B	4.06	126.66	116.53
9	B	605	HEM	CMC-C2C-C3C	4.69	128.24	116.53
9	A	605	HEM	CMC-C2C-C3C	4.71	128.28	116.53
9	A	605	HEM	CAD-C3D-C2D	5.05	127.73	113.22
9	B	605	HEM	CAD-C3D-C2D	5.10	127.88	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	605	HEM	3	0
9	B	605	HEM	2	0
8	C	1606	ACT	4	0
4	C	1620	NAG	1	0
8	D	2604	ACT	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 ⓘ

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	104/104 (100%)	1.41	19 (18%) 2 3	2, 6, 17, 43	0
1	B	104/104 (100%)	1.47	28 (26%) 1 1	3, 7, 15, 23	0
2	C	465/466 (99%)	1.50	113 (24%) 1 1	2, 7, 19, 35	0
2	D	465/466 (99%)	1.67	145 (31%) 1 1	3, 9, 24, 41	0
All	All	1138/1140 (99%)	1.56	305 (26%) 1 1	2, 8, 22, 43	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	14.8
2	D	355	PRO	8.9
2	D	568	PRO	6.2
1	A	4	GLN	5.8
2	D	578	ALA	5.3
1	A	2	PRO	5.2
2	C	353	MET	5.1
2	D	218	ASP	5.0
2	D	543	ILE	5.0
2	C	223	LEU	5.0
2	C	355	PRO	4.9
2	D	562	VAL	4.7
2	D	217	HIS	4.6
2	C	190	MET	4.5
2	C	157	ASN	4.4
2	D	529	ALA	4.3
2	C	212	PRO	4.3
2	C	158	ILE	4.2
2	D	575	TRP	4.1
2	C	199	VAL	4.1
1	A	1	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	1	CYS	4.1
2	D	261	ALA	4.0
2	D	113	VAL	4.0
2	D	315	SER	3.9
2	C	351	GLN	3.8
2	C	155	GLY	3.7
1	A	3	GLU	3.7
2	D	216	LEU	3.7
2	D	222	LEU	3.7
2	D	351	GLN	3.7
2	D	572	LEU	3.7
2	D	269	PRO	3.7
2	D	406	LEU	3.6
2	D	417	LEU	3.6
2	C	217	HIS	3.6
1	A	97	LEU	3.6
1	B	89	TRP	3.6
2	D	227	SER	3.6
2	D	190	MET	3.6
2	C	452	GLY	3.6
2	D	226	ARG	3.5
1	B	60	LEU	3.5
2	D	538	CYS	3.5
2	D	157	ASN	3.5
2	C	147	PHE	3.5
1	B	47	TRP	3.5
2	C	436	TRP	3.5
2	D	124	PRO	3.5
2	D	527	ALA	3.5
2	D	202	ARG	3.4
2	D	407	PHE	3.4
2	D	303	PRO	3.4
2	C	141	ALA	3.4
2	C	578	ALA	3.4
2	D	352	PRO	3.4
2	D	267	LEU	3.3
2	D	253	LEU	3.3
2	C	379	PRO	3.3
2	D	117	THR	3.3
2	D	328	PHE	3.3
2	C	128	LEU	3.2
1	B	51	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	357	PRO	3.2
2	C	324	ILE	3.1
2	C	369	TRP	3.1
2	D	567	LEU	3.1
2	D	173	ALA	3.1
2	D	185	ARG	3.1
2	D	471	PRO	3.1
2	C	561	PHE	3.1
2	D	360	PRO	3.0
2	D	302	GLY	3.0
2	D	557	TYR	3.0
2	D	271	TRP	3.0
2	D	410	VAL	3.0
1	B	33	LEU	3.0
2	D	264	LEU	3.0
2	C	557	TYR	3.0
2	D	357	PRO	3.0
2	C	327	VAL	3.0
2	C	359	VAL	3.0
1	B	63	ALA	3.0
2	C	133	ASN	2.9
1	B	92	LEU	2.9
2	D	272	ASP	2.9
2	D	348	ASN	2.9
2	D	499	ILE	2.9
2	C	216	LEU	2.9
2	D	576	ARG	2.9
2	D	309	TYR	2.9
2	C	543	ILE	2.9
2	D	546	VAL	2.9
2	D	542	GLY	2.9
2	D	296	TYR	2.9
1	A	30	VAL	2.9
2	D	212	PRO	2.8
2	D	164	ILE	2.8
2	C	417	LEU	2.8
2	C	462	ARG	2.8
2	C	114	ASN	2.8
2	D	356	ASN	2.8
1	A	47	TRP	2.8
2	D	561	PHE	2.8
2	D	566	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	140	GLN	2.8
2	C	440	CYS	2.8
2	C	139	ASN	2.8
2	D	359	VAL	2.8
2	D	494	LEU	2.8
2	C	519	VAL	2.8
2	D	419	ALA	2.7
2	C	211	LEU	2.7
2	C	506	LEU	2.7
2	C	354	GLU	2.7
2	C	328	PHE	2.7
1	A	89	TRP	2.7
2	D	574	SER	2.7
2	C	320	VAL	2.7
2	D	120	VAL	2.7
2	C	283	ILE	2.7
2	D	350	TYR	2.7
1	A	76	LEU	2.7
2	C	352	PRO	2.7
2	C	171	VAL	2.7
2	C	313	TYR	2.7
2	D	397	ILE	2.7
2	D	485	LEU	2.7
2	D	353	MET	2.6
1	A	93	LEU	2.6
2	D	220	PRO	2.6
2	D	221	CYS	2.6
2	D	544	THR	2.6
2	C	461	ALA	2.6
2	D	176	VAL	2.6
2	D	147	PHE	2.6
1	B	100	THR	2.6
2	C	253	LEU	2.6
2	C	430	LEU	2.6
2	C	485	LEU	2.6
2	C	386	ALA	2.6
2	D	280	ALA	2.6
2	C	419	ALA	2.6
2	C	220	PRO	2.6
2	C	477	TRP	2.6
1	A	99	PHE	2.6
2	C	325	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	496	ALA	2.6
2	C	264	LEU	2.6
2	C	334	TYR	2.6
2	D	156	SER	2.5
2	D	565	SER	2.5
2	D	325	ALA	2.5
2	D	558	PRO	2.5
1	B	97	LEU	2.5
2	D	155	GLY	2.5
2	D	246	LEU	2.5
2	D	192	ASN	2.5
1	A	41	PHE	2.5
2	C	332	PHE	2.5
2	D	548	LYS	2.5
1	B	28	ALA	2.5
2	C	558	PRO	2.5
2	D	436	TRP	2.5
2	D	545	THR	2.5
2	C	203	PHE	2.5
2	C	246	LEU	2.5
2	D	233	PHE	2.5
2	D	455	LEU	2.5
1	A	92	LEU	2.5
2	D	211	LEU	2.5
2	D	254	LEU	2.5
2	D	339	ILE	2.5
1	A	32	TRP	2.5
2	D	191	SER	2.5
2	D	193	GLN	2.5
2	D	292	THR	2.4
2	D	207	GLY	2.4
2	D	125	CYS	2.4
2	D	169	SER	2.4
2	C	458	LEU	2.4
2	D	290	ILE	2.4
1	A	29	PHE	2.4
1	A	71	PHE	2.4
2	C	513	TRP	2.4
2	D	369	TRP	2.4
2	C	329	THR	2.4
2	D	337	THR	2.4
2	D	266	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	522	MET	2.4
2	D	498	ILE	2.4
2	C	127	PRO	2.4
2	C	542	GLY	2.4
1	B	32	TRP	2.4
2	C	514	TRP	2.4
2	D	399	VAL	2.4
2	C	349	ARG	2.4
2	C	176	VAL	2.4
2	D	300	VAL	2.4
2	D	349	ARG	2.4
1	B	83	SER	2.4
2	D	379	PRO	2.4
1	B	84	LEU	2.3
2	C	130	ILE	2.3
2	C	125	CYS	2.3
2	D	310	LEU	2.3
2	C	170	PHE	2.3
2	C	552	PHE	2.3
2	C	304	THR	2.3
2	C	576	ARG	2.3
2	C	227	SER	2.3
2	C	276	LEU	2.3
2	D	234	LEU	2.3
2	C	476	ILE	2.3
2	D	476	ILE	2.3
2	D	354	GLU	2.3
2	D	520	PHE	2.3
2	C	448	VAL	2.3
2	D	223	LEU	2.3
2	C	537	ILE	2.3
2	C	213	PHE	2.3
2	D	314	ARG	2.3
1	B	30	VAL	2.3
2	D	492	GLY	2.3
1	B	14	CYS	2.3
2	C	221	CYS	2.3
2	C	538	CYS	2.3
2	C	409	GLN	2.3
2	C	173	ALA	2.2
1	B	64	VAL	2.2
1	B	78	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	99	PHE	2.2
2	D	225	ASN	2.2
2	D	381	LEU	2.2
1	B	45	TYR	2.2
1	A	86	PHE	2.2
2	C	365	PHE	2.2
2	C	285	GLY	2.2
1	B	43	LEU	2.2
1	B	49	PRO	2.2
2	C	391	LEU	2.2
2	C	568	PRO	2.2
2	D	373	LEU	2.2
2	C	228	ALA	2.2
2	C	398	ALA	2.2
2	D	262	THR	2.2
2	C	331	ALA	2.2
2	D	331	ALA	2.2
2	C	284	VAL	2.2
2	D	201	GLN	2.2
2	D	154	PRO	2.1
2	D	182	PRO	2.1
2	D	203	PHE	2.1
1	B	93	LEU	2.1
2	C	194	LEU	2.1
2	C	196	LEU	2.1
2	D	430	LEU	2.1
2	D	563	ASN	2.1
2	C	529	ALA	2.1
2	D	402	ILE	2.1
2	D	270	ARG	2.1
2	D	547	SER	2.1
2	C	366	PHE	2.1
2	C	512	PHE	2.1
2	C	545	THR	2.1
2	D	210	LEU	2.1
2	D	252	LEU	2.1
2	D	338	LEU	2.1
2	C	198	ALA	2.1
2	C	218	ASP	2.1
2	D	174	SER	2.1
2	C	350	TYR	2.1
2	C	209	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	555	ASN	2.1
1	A	68	ILE	2.1
2	D	564	CYS	2.1
2	D	559	ARG	2.1
2	D	284	VAL	2.1
2	C	309	TYR	2.1
2	C	316	TYR	2.1
2	D	287	MET	2.1
1	B	71	PHE	2.1
2	C	344	PHE	2.1
2	D	366	PHE	2.1
2	D	276	LEU	2.1
2	D	377	ILE	2.1
1	B	69	VAL	2.0
1	B	73	THR	2.0
1	B	56	PHE	2.0
2	D	332	PHE	2.0
2	D	342	PHE	2.0
2	C	260	LEU	2.0
2	D	268	ASN	2.0
2	C	291	ILE	2.0
1	A	5	ASP	2.0
2	D	327	VAL	2.0
2	C	305	ALA	2.0
2	C	564	CYS	2.0
2	D	286	ALA	2.0
1	B	41	PHE	2.0
2	C	338	LEU	2.0
2	C	415	LEU	2.0
2	C	464	LEU	2.0
2	D	570	LEU	2.0
2	C	450	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSO	D	150	7/8	0.91	0.13	-	5,6,8,10	0
2	CSO	C	150	7/8	0.94	0.10	-	2,5,7,9	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	C	1642	11/12	0.84	0.22	2.75	9,14,15,18	0
3	BMA	D	2642	11/12	0.87	0.17	1.22	9,12,14,18	0
3	NAG	C	1641	14/15	0.88	0.17	0.47	5,8,11,12	0
3	NAG	D	2641	14/15	0.91	0.13	-0.33	6,8,10,11	0
3	NAG	C	1640	14/15	0.89	0.14	-	6,8,11,13	0
3	MAN	D	2644	11/12	0.82	0.22	-	9,14,18,23	0
3	NAG	D	2640	14/15	0.88	0.15	-	9,10,15,16	0
3	FUC	C	1645	10/11	0.85	0.14	-	9,13,15,17	0
3	MAN	C	1644	11/12	0.86	0.18	-	13,15,17,18	0
3	MAN	C	1643	11/12	0.80	0.23	-	21,25,26,28	0
3	FUC	D	2645	10/11	0.79	0.22	-	10,14,16,19	0
3	MAN	D	2643	11/12	0.68	0.26	-	17,20,22,23	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	ACT	C	1606	4/4	0.47	0.27	6.82	22,23,24,25	0
4	NAG	C	1630	14/15	0.74	0.23	1.84	18,22,27,28	0
4	NAG	D	2620	14/15	0.79	0.24	1.44	16,21,26,28	0
4	NAG	D	2630	14/15	0.75	0.25	1.34	26,30,34,35	0
4	NAG	C	1620	14/15	0.86	0.21	1.16	9,14,20,24	0
9	HEM	A	605	43/43	0.94	0.17	-0.18	2,5,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	HEM	B	605	43/43	0.93	0.16	-0.49	2,5,8,9	0
8	ACT	D	2606	4/4	0.91	0.12	-0.58	13,14,14,18	0
5	CA	B	600	1/1	1.00	0.13	-2.08	7,7,7,7	0
6	BR	B	889	1/1	0.98	0.06	-2.13	23,23,23,23	1
5	CA	A	600	1/1	1.00	0.10	-2.77	5,5,5,5	0
6	BR	A	889	1/1	0.99	0.06	-2.97	24,24,24,24	1
6	BR	B	758	1/1	0.94	0.12	-3.02	18,18,18,18	1
6	BR	B	601	1/1	1.00	0.10	-3.84	6,6,6,6	0
6	BR	A	758	1/1	0.98	0.07	-5.08	16,16,16,16	1
6	BR	A	601	1/1	1.00	0.09	-5.62	6,6,6,6	0
8	ACT	C	1607	4/4	0.79	0.26	-	22,23,23,25	0
8	ACT	D	2604	4/4	0.64	0.43	-	32,34,34,34	0
8	ACT	D	2607	4/4	0.48	0.29	-	29,30,30,31	0
6	BR	A	843	1/1	0.97	0.14	-	12,12,12,12	1
7	SO4	C	1603	5/5	0.93	0.12	-	20,21,23,25	0
7	SO4	B	2602	5/5	0.48	0.33	-	42,42,43,44	5
8	ACT	C	1604	4/4	0.73	0.23	-	17,17,20,22	0
7	SO4	A	1602	5/5	0.96	0.10	-	19,19,21,22	0
6	BR	B	843	1/1	0.99	0.06	-	12,12,12,12	1

6.5 Other polymers [i](#)

There are no such residues in this entry.