



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:54 PM EDT

PDB ID : 3EDX  
Title : Crystal structure of the W215A/E217A mutant of murine thrombin  
Authors : Gandhi, P.S.; Page, M.J.; Chen, Z.; Bush-pelc, L.; Di Cera, E.  
Deposited on : 2008-09-03  
Resolution : 2.40 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](mailto: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.

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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 : 2.23.2  
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) : 2.23.2

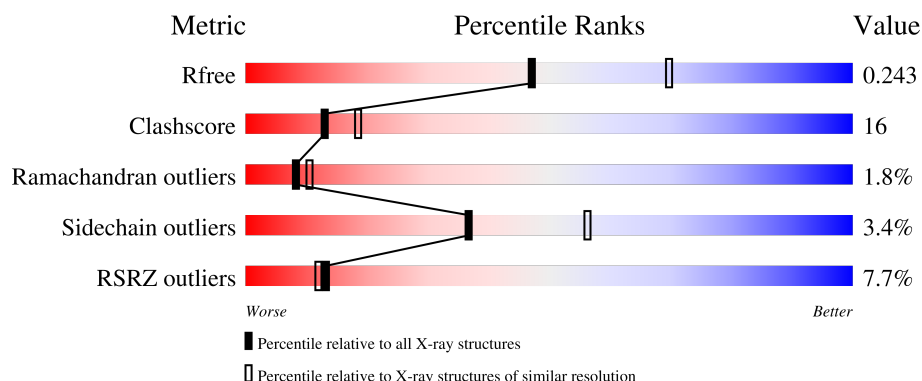
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	44	
1	C	44	
1	E	44	
2	B	258	
2	D	258	

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Mol	Chain	Length	Quality of chain
2	F	258	 A horizontal bar chart showing the quality of chain F. The bar is divided into segments: a small red segment at the beginning labeled '6%', followed by a long green segment labeled '60%', then a yellow segment labeled '36%', and a very small orange segment at the end. A small black dot is visible at the far right end of the bar.

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
4	NAG	D	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7612 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	42	Total	C	N	O	S	0	0	0
			339	219	51	68	1			
1	C	42	Total	C	N	O	S	0	0	0
			339	219	51	68	1			
1	E	42	Total	C	N	O	S	0	0	0
			339	219	51	68	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2097	1342	377	366	12			
2	D	258	Total	C	N	O	S	0	0	0
			2097	1342	377	366	12			
2	F	258	Total	C	N	O	S	0	0	0
			2097	1342	377	366	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	ALA	TRP	engineered mutation	UNP P19221
B	217	ALA	GLU	engineered mutation	UNP P19221
D	215	ALA	TRP	engineered mutation	UNP P19221
D	217	ALA	GLU	engineered mutation	UNP P19221
F	215	ALA	TRP	engineered mutation	UNP P19221
F	217	ALA	GLU	engineered mutation	UNP P19221

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	78	Total	O	0	0
			78	78		
5	C	8	Total	O	0	0
			8	8		
5	D	52	Total	O	0	0
			52	52		
5	E	10	Total	O	0	0
			10	10		
5	F	57	Total	O	0	0
			57	57		

### 3 Residue-property plots [i](#)


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

- Molecule 1: Thrombin light chain

Chain A: 



- Molecule 1: Thrombin light chain

Chain C: 



- Molecule 1: Thrombin light chain

Chain E: 

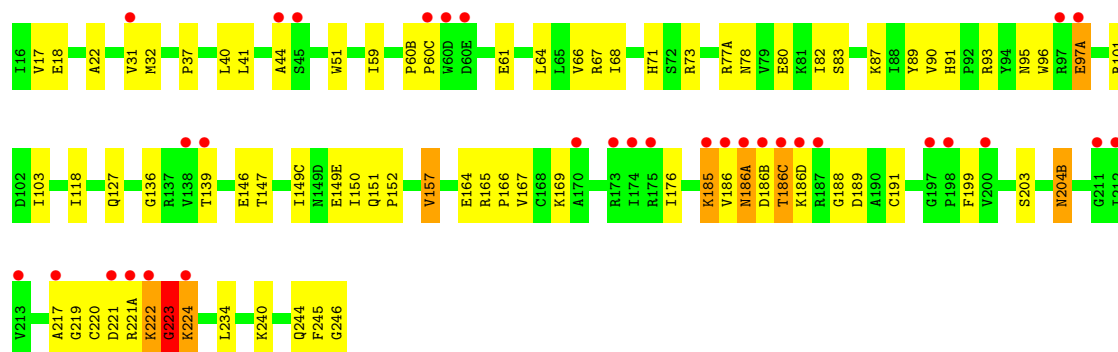


- Molecule 2: Thrombin heavy chain

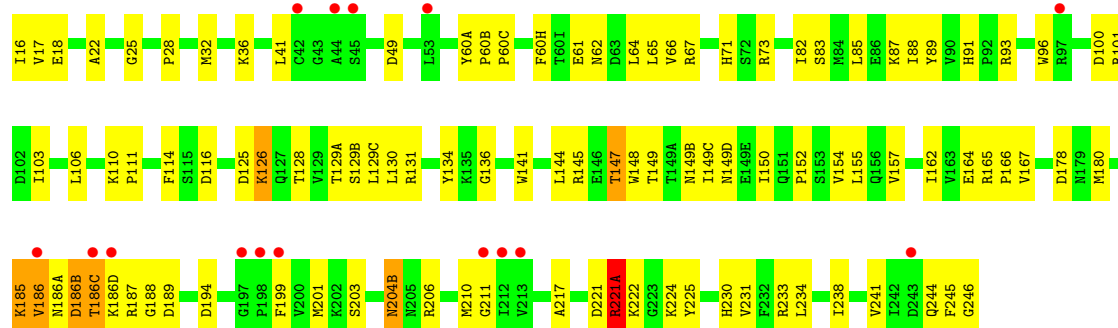
Chain B: 



- Molecule 2: Thrombin heavy chain



• Molecule 2: Thrombin heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.72Å 105.76Å 176.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.78 – 2.40 32.78 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.78-2.40) 92.3 (32.78-2.41)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.214 , 0.243 0.214 , 0.243	Depositor DCC
$R_{free}$ test set	3447 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, 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	0.41	0/345	0.66	0/461
1	C	0.41	0/345	0.65	0/461
1	E	0.41	0/345	0.65	0/461
2	B	0.39	0/2152	0.65	0/2913
2	D	0.37	0/2152	0.65	1/2913 (0.0%)
2	F	0.42	2/2152 (0.1%)	0.64	0/2913
All	All	0.39	2/7491 (0.0%)	0.65	1/10122 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	221(A)	ARG	CG-CD	-6.06	1.36	1.51
2	F	221(A)	ARG	CB-CG	-6.04	1.36	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	GLY	N-CA-C	5.61	127.13	113.10

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	339	0	328	6	0
1	C	339	0	328	4	0
1	E	339	0	328	9	0
2	B	2097	0	2096	75	0
2	D	2097	0	2096	69	0
2	F	2097	0	2096	91	0
3	B	10	0	0	0	0
3	D	15	0	0	0	0
3	F	10	0	0	1	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
5	A	22	0	0	2	0
5	B	78	0	0	3	0
5	C	8	0	0	0	0
5	D	52	0	0	2	0
5	E	10	0	0	1	0
5	F	57	0	0	7	0
All	All	7612	0	7311	241	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 16.

All (241) 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:185:LYS:HE3	2:B:185:LYS:HA	1.60	0.83
1:E:14(K):ILE:O	1:E:14(L):ASP:HB2	1.78	0.83
2:D:186(C):THR:HG23	2:D:186(D):LYS:H	1.43	0.83
2:F:186(C):THR:HG23	2:F:186(D):LYS:H	1.43	0.82
2:F:149(B):ASN:HD21	2:F:149(D):ASN:HB2	1.45	0.81
2:D:67:ARG:HD3	2:D:82:ILE:HD12	1.67	0.77
2:B:147:THR:HG22	2:B:221:ASP:OD1	1.86	0.76
2:B:89:TYR:CE2	2:B:246:GLY:HA3	2.19	0.76
2:F:89:TYR:CE2	2:F:246:GLY:HA3	2.23	0.73
2:B:221(A):ARG:NH2	2:F:148:TRP:HE1	1.86	0.72
2:F:67:ARG:HD3	2:F:82:ILE:HD12	1.70	0.72
2:B:186(C):THR:HG23	2:B:186(D):LYS:N	2.05	0.70
2:F:221(A):ARG:NE	5:F:460:HOH:O	2.26	0.68
2:D:18:GLU:HB2	2:D:188:GLY:HA2	1.74	0.68
2:F:149(B):ASN:ND2	2:F:149(D):ASN:HB2	2.09	0.67
2:F:130:LEU:HD12	2:F:162:ILE:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186(A):ASN:O	2:B:186(C):THR:N	2.28	0.65
1:E:10:LYS:O	1:E:12:LEU:HD13	1.97	0.65
2:D:164:GLU:HB2	2:D:167:VAL:CG2	2.26	0.65
2:D:176:ILE:HG13	2:D:176:ILE:O	1.97	0.65
2:F:17:VAL:HG12	2:F:18:GLU:HG2	1.77	0.64
2:F:130:LEU:HD12	2:F:162:ILE:CD1	2.28	0.64
2:D:221:ASP:C	2:D:222:LYS:H	2.01	0.64
2:B:186(C):THR:CG2	2:B:186(D):LYS:H	2.11	0.64
2:D:73:ARG:HD3	2:D:152:PRO:O	1.98	0.64
2:F:36:LYS:HD2	2:F:62:ASN:O	1.96	0.63
2:F:103:ILE:HG21	2:F:234:LEU:HD13	1.80	0.63
2:B:147:THR:HG22	2:B:221:ASP:CG	2.17	0.63
2:B:185:LYS:HD2	2:D:37:PRO:HD3	1.80	0.63
2:F:60(B):PRO:HB2	2:F:60(C):PRO:HD3	1.79	0.63
2:B:185:LYS:HE2	2:B:225:TYR:OH	1.98	0.63
2:D:89:TYR:CE2	2:D:246:GLY:HA3	2.34	0.63
2:B:74:THR:HG22	5:B:465:HOH:O	1.99	0.63
1:E:6:LEU:HD21	2:F:116:ASP:HB3	1.80	0.62
2:F:61:GLU:H	2:F:61:GLU:CD	2.02	0.62
2:B:186(C):THR:CG2	2:B:186(D):LYS:N	2.62	0.61
2:D:223:GLY:O	2:D:224:LYS:HG2	2.00	0.61
2:B:148:TRP:HE1	2:F:221(A):ARG:NH2	1.99	0.61
2:B:244:GLN:O	2:B:245:PHE:HB2	2.02	0.60
2:F:164:GLU:HB2	2:F:167:VAL:CG2	2.31	0.60
2:F:18:GLU:HB2	2:F:188:GLY:HA2	1.84	0.60
2:F:224:LYS:HE2	5:F:442:HOH:O	2.00	0.60
2:D:95:ASN:HD22	2:D:97(A):GLU:HB2	1.66	0.60
2:B:185:LYS:HA	2:B:185:LYS:CE	2.31	0.59
2:B:221(A):ARG:HH22	2:F:148:TRP:HE1	1.51	0.59
2:B:17:VAL:HG12	2:B:18:GLU:HG2	1.85	0.58
2:B:91:HIS:CE1	2:B:101:ARG:HD3	2.38	0.58
2:F:136:GLY:HA3	2:F:199:PHE:CZ	2.39	0.58
2:B:185:LYS:HE3	2:B:185:LYS:CA	2.32	0.58
2:D:67:ARG:HD3	2:D:82:ILE:CD1	2.33	0.58
2:B:22:ALA:O	2:B:71:HIS:HE1	1.86	0.58
2:B:61:GLU:CD	2:B:61:GLU:H	2.07	0.58
2:D:17:VAL:HG12	2:D:18:GLU:HG2	1.86	0.57
2:F:49:ASP:HB3	2:F:114:PHE:CZ	2.39	0.57
2:F:164:GLU:HB2	2:F:167:VAL:HG23	1.87	0.57
2:D:127:GLN:HG3	5:D:438:HOH:O	2.06	0.56
2:B:186(C):THR:HG23	2:B:186(D):LYS:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:91:HIS:CE1	2:F:93:ARG:HB2	2.40	0.56
2:B:73:ARG:HD3	2:B:152:PRO:O	2.05	0.56
2:F:25:GLY:O	2:F:28:PRO:HD3	2.06	0.56
2:D:61:GLU:CD	2:D:61:GLU:H	2.08	0.55
2:F:211:GLY:HA2	2:F:231:VAL:HG23	1.87	0.55
2:D:165:ARG:HB3	2:D:166:PRO:HD3	1.87	0.55
2:F:66:VAL:HG13	2:F:85:LEU:HD21	1.87	0.55
1:A:14(A):THR:HG22	1:A:14(B):THR:HG23	1.88	0.55
2:D:245:PHE:O	2:D:246:GLY:O	2.23	0.55
2:B:53:LEU:HG	2:B:212:ILE:HD11	1.88	0.55
2:F:147:THR:O	2:F:148:TRP:HB2	2.05	0.55
1:C:10:LYS:O	1:C:12:LEU:HD13	2.07	0.55
2:D:219:GLY:O	2:D:220:CYS:HB2	2.07	0.55
2:F:22:ALA:O	2:F:71:HIS:HE1	1.90	0.55
2:B:41:LEU:HD11	2:B:60(H):PHE:CE2	2.42	0.54
2:D:146:GLU:HG2	2:D:147:THR:HG23	1.88	0.54
2:B:165:ARG:HB3	2:B:166:PRO:HD3	1.89	0.54
1:E:14(D):LYS:HE2	1:E:14(H):ASP:OD1	2.08	0.54
2:B:17:VAL:HG23	2:B:191:CYS:SG	2.48	0.54
2:D:103:ILE:HG21	2:D:234:LEU:HD13	1.90	0.53
2:B:67:ARG:HD3	2:B:82:ILE:HD12	1.89	0.53
2:B:186(C):THR:HG23	2:B:186(D):LYS:HG3	1.89	0.53
2:D:240:LYS:HE3	5:D:444:HOH:O	2.07	0.53
2:B:103:ILE:HG21	2:B:234:LEU:HD13	1.91	0.53
2:D:186(C):THR:HG23	2:D:186(D):LYS:N	2.21	0.53
2:F:91:HIS:CE1	2:F:101:ARG:HD3	2.44	0.53
2:B:147:THR:O	2:B:148:TRP:HB2	2.09	0.53
2:F:32:MET:HB2	2:F:141:TRP:CZ3	2.43	0.52
2:F:61:GLU:HG3	2:F:87:LYS:HA	1.91	0.52
2:D:217:ALA:HB1	2:D:223:GLY:HA3	1.91	0.52
2:D:149(E):GLU:HG3	2:D:150:ILE:HG23	1.92	0.52
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HB2	2.45	0.52
2:D:60(B):PRO:HB2	2:D:60(C):PRO:HD3	1.92	0.52
1:C:14(A):THR:HG22	1:C:14(B):THR:HG23	1.92	0.51
2:D:221(A):ARG:O	2:D:222:LYS:HB2	2.11	0.51
2:F:185:LYS:HE3	2:F:185:LYS:HA	1.92	0.51
2:D:185:LYS:HE3	2:D:185:LYS:N	2.25	0.51
2:F:165:ARG:HB3	2:F:166:PRO:HD3	1.92	0.51
1:C:13:LYS:HA	1:C:14(C):GLU:OE2	2.11	0.51
2:F:100:ASP:HA	2:F:180:MET:CE	2.41	0.51
2:D:67:ARG:HD2	2:D:80:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLY:HA3	2:D:199:PHE:CZ	2.46	0.51
2:B:60(A):TYR:CE1	2:F:148:TRP:CH2	2.99	0.51
2:D:41:LEU:CD1	2:D:64:LEU:HD22	2.41	0.51
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	1.93	0.51
2:F:185:LYS:O	2:F:186(A):ASN:N	2.45	0.50
2:F:244:GLN:O	2:F:245:PHE:HB2	2.11	0.50
2:F:149(B):ASN:HD21	2:F:149(D):ASN:HD22	1.59	0.50
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.10	0.50
2:F:178:ASP:O	2:F:233:ARG:HD3	2.10	0.50
2:D:203:SER:HB3	2:D:204(B):ASN:HD21	1.77	0.49
5:B:455:HOH:O	2:F:222:LYS:HD3	2.12	0.49
2:B:18:GLU:HB2	2:B:188:GLY:HA2	1.94	0.49
2:F:185:LYS:HE2	2:F:225:TYR:OH	2.12	0.49
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.94	0.49
2:F:61:GLU:CG	2:F:87:LYS:HA	2.43	0.49
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.15	0.49
2:F:203:SER:HB3	2:F:204(B):ASN:ND2	2.28	0.49
2:B:149:THR:O	2:B:149(A):THR:HB	2.13	0.48
2:D:61:GLU:CG	2:D:87:LYS:HA	2.43	0.48
2:D:51:TRP:HZ2	2:D:245:PHE:CD1	2.31	0.48
2:F:60(C):PRO:HD3	2:F:96:TRP:CZ3	2.48	0.48
2:B:220:CYS:HB2	5:B:460:HOH:O	2.12	0.48
2:D:185:LYS:O	2:D:186(A):ASN:N	2.47	0.48
2:D:164:GLU:HB2	2:D:167:VAL:HG23	1.94	0.48
2:B:169:LYS:HA	2:B:176:ILE:HD12	1.95	0.48
2:B:36:LYS:HE2	2:B:84:MET:HE1	1.95	0.48
2:D:165:ARG:O	2:D:169:LYS:HG3	2.14	0.48
2:D:146:GLU:HB2	2:D:220:CYS:C	2.34	0.47
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.96	0.47
2:F:144:LEU:HD21	2:F:152:PRO:HB3	1.97	0.47
1:C:14(D):LYS:HE2	1:C:14(H):ASP:OD1	2.14	0.47
2:D:169:LYS:CG	2:D:176:ILE:HD11	2.44	0.47
2:F:149(B):ASN:HD21	2:F:149(D):ASN:CB	2.23	0.47
2:B:32:MET:HE2	2:B:141:TRP:CD2	2.50	0.47
2:F:18:GLU:OE1	2:F:186(D):LYS:HE3	2.15	0.47
2:D:223:GLY:O	2:D:224:LYS:CB	2.63	0.47
2:D:139:THR:HG22	2:D:157:VAL:HB	1.96	0.46
2:B:84:MET:HB2	2:B:109:LYS:HD2	1.98	0.46
2:B:222:LYS:HD2	5:F:443:HOH:O	2.15	0.46
2:D:32:MET:HG3	2:D:40:LEU:HD13	1.96	0.46
2:D:68:ILE:HG22	2:D:118:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:SER:HB3	2:D:204(B):ASN:ND2	2.31	0.46
2:F:66:VAL:CG1	2:F:85:LEU:HD21	2.45	0.46
2:D:221:ASP:O	2:D:222:LYS:N	2.43	0.46
1:E:14(L):ASP:HA	2:F:134:TYR:OH	2.15	0.46
2:F:110:LYS:HE2	5:F:436:HOH:O	2.14	0.46
2:F:189:ASP:OD2	2:F:217:ALA:HB3	2.16	0.46
1:A:14(D):LYS:HB2	5:A:29:HOH:O	2.16	0.46
2:D:221(A):ARG:O	2:D:221(A):ARG:HD2	2.15	0.46
1:E:5:PRO:HB2	2:F:116:ASP:HA	1.98	0.46
2:D:91:HIS:CE1	2:D:101:ARG:HD3	2.51	0.46
2:D:93:ARG:NH2	2:D:101:ARG:NH2	2.64	0.46
2:B:32:MET:HE2	2:B:141:TRP:CE3	2.50	0.46
2:F:154:VAL:CG1	2:F:155:LEU:N	2.79	0.46
2:B:221(A):ARG:NH2	2:F:148:TRP:NE1	2.58	0.45
2:D:60(B):PRO:HG2	2:D:96:TRP:CZ2	2.52	0.45
1:A:13:LYS:HD2	5:A:30:HOH:O	2.14	0.45
2:F:41:LEU:HD11	2:F:60(H):PHE:CE2	2.51	0.45
2:F:125:ASP:HB2	3:F:301:SO4:O2	2.15	0.45
2:F:16:ILE:N	2:F:194:ASP:OD2	2.50	0.45
2:B:222:LYS:NZ	2:B:222:LYS:HB3	2.31	0.45
2:F:65:LEU:HD12	2:F:65:LEU:C	2.37	0.45
1:A:10:LYS:O	1:A:12:LEU:HD13	2.17	0.44
2:B:100:ASP:HA	2:B:180:MET:CE	2.46	0.44
2:B:60(B):PRO:HD2	2:B:96:TRP:CD2	2.52	0.44
2:D:169:LYS:HG3	2:D:176:ILE:HD11	1.99	0.44
2:F:186(C):THR:HG23	2:F:186(D):LYS:N	2.22	0.44
2:D:221(A):ARG:O	2:D:222:LYS:CB	2.65	0.44
2:F:49:ASP:O	2:F:111:PRO:HA	2.17	0.44
2:F:126:LYS:O	2:F:129(A):THR:HG23	2.17	0.44
2:B:36(A):SER:HA	2:B:37:PRO:C	2.38	0.44
2:B:93:ARG:NH2	2:B:101:ARG:NH2	2.66	0.43
1:E:1(C):GLU:HB2	5:E:173:HOH:O	2.18	0.43
2:F:149(C):ILE:HD12	2:F:150:ILE:HD11	1.99	0.43
2:F:221(A):ARG:HD3	5:F:460:HOH:O	2.18	0.43
2:B:60(A):TYR:CE1	2:F:148:TRP:HH2	2.36	0.43
2:F:66:VAL:CG2	2:F:83:SER:HB2	2.48	0.43
2:F:147:THR:CG2	2:F:221:ASP:OD2	2.66	0.43
2:F:203:SER:HB3	2:F:204(B):ASN:HD21	1.82	0.43
1:A:14(K):ILE:O	1:A:14(L):ASP:C	2.57	0.43
2:B:178:ASP:HB2	2:B:233:ARG:HH21	1.83	0.43
2:D:221:ASP:C	2:D:222:LYS:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:GLN:O	2:D:245:PHE:HB2	2.19	0.43
2:D:146:GLU:HB2	2:D:220:CYS:O	2.18	0.43
2:F:73:ARG:HD3	2:F:152:PRO:O	2.19	0.43
2:F:185:LYS:O	2:F:187:ARG:HD3	2.18	0.43
2:B:201:MET:SD	2:B:210:MET:HG3	2.59	0.43
2:F:87:LYS:HG3	2:F:88:ILE:H	1.84	0.43
2:D:17:VAL:HG23	2:D:191:CYS:SG	2.58	0.43
2:F:131:ARG:O	2:F:134:TYR:HB2	2.18	0.43
1:E:1(K):ASN:OD1	1:E:1(I):LYS:HB2	2.18	0.42
2:B:49:ASP:HB3	2:B:114:PHE:CZ	2.54	0.42
2:F:147:THR:O	2:F:148:TRP:CB	2.68	0.42
2:F:204(B):ASN:ND2	2:F:206:ARG:H	2.18	0.42
2:B:36:LYS:HE2	2:B:84:MET:CE	2.50	0.42
2:D:17:VAL:O	2:D:188:GLY:HA2	2.20	0.42
2:D:186(A):ASN:O	2:D:186(C):THR:N	2.53	0.42
2:F:186(B):ASP:HB3	5:F:450:HOH:O	2.19	0.42
2:B:99:LEU:O	2:B:102:ASP:HB2	2.20	0.42
2:B:186:VAL:O	2:B:186:VAL:HG23	2.19	0.42
2:B:147:THR:O	2:B:148:TRP:CB	2.68	0.42
2:D:77(A):ARG:O	2:D:78:ASN:HB2	2.19	0.42
2:F:18:GLU:HB2	2:F:188:GLY:CA	2.50	0.42
2:F:221(A):ARG:CD	5:F:460:HOH:O	2.67	0.42
2:B:17:VAL:O	2:B:188:GLY:HA2	2.20	0.42
2:B:121:VAL:HG22	2:B:122:CYS:N	2.35	0.42
2:B:185:LYS:HD2	2:D:37:PRO:CD	2.46	0.42
2:D:51:TRP:HZ2	2:D:245:PHE:HD1	1.68	0.42
2:F:234:LEU:O	2:F:238:ILE:HG13	2.20	0.42
2:D:136:GLY:HA3	2:D:199:PHE:CE1	2.55	0.41
2:B:65:LEU:HD13	2:B:82:ILE:HG23	2.02	0.41
2:B:74:THR:HG23	2:B:75:ARG:H	1.85	0.41
2:D:59:ILE:N	2:D:59:ILE:HD12	2.35	0.41
1:A:4:ARG:HA	1:A:5:PRO:HD3	1.88	0.41
2:B:148:TRP:HE1	2:F:221(A):ARG:HH22	1.67	0.41
2:D:66:VAL:CG2	2:D:83:SER:HB2	2.50	0.41
2:F:201:MET:SD	2:F:210:MET:HG3	2.61	0.41
2:D:32:MET:HG3	2:D:40:LEU:CD1	2.50	0.41
2:F:128:THR:HG23	2:F:129(C):LEU:HD12	2.02	0.41
2:F:186:VAL:O	2:F:186:VAL:HG22	2.20	0.41
2:F:230:HIS:CG	2:F:233:ARG:HG3	2.56	0.41
2:D:95:ASN:ND2	2:D:97(A):GLU:H	2.19	0.41
2:F:241:VAL:O	2:F:245:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:ALA:O	2:D:71:HIS:HE1	2.04	0.41
2:D:151:GLN:HE21	2:D:151:GLN:HB3	1.65	0.41
2:D:188:GLY:O	2:D:189:ASP:HB2	2.21	0.41
2:B:65:LEU:HD12	2:B:65:LEU:C	2.42	0.40
2:B:148:TRP:CH2	2:F:60(A):TYR:CE1	3.08	0.40
1:E:4:ARG:HA	1:E:5:PRO:HD3	1.97	0.40
2:F:148:TRP:HA	2:F:148:TRP:CE3	2.56	0.40
2:F:185:LYS:HA	2:F:185:LYS:CE	2.50	0.40
2:B:197:GLY:O	2:B:213:VAL:HG23	2.22	0.40
2:D:165:ARG:HG2	2:D:169:LYS:HE3	2.03	0.40
2:F:87:LYS:HG3	2:F:88:ILE:N	2.36	0.40
2:F:88:ILE:HG23	2:F:106:LEU:CD2	2.50	0.40
2:F:145:ARG:HH21	2:F:149:THR:HB	1.86	0.40
2:B:32:MET:SD	2:B:34:PHE:CE2	3.15	0.40
2:B:68:ILE:O	2:B:80:GLU:HA	2.22	0.40
2:B:74:THR:HG23	2:B:75:ARG:N	2.36	0.40
2:B:34:PHE:HD2	2:B:67:ARG:HG3	1.87	0.40
2:B:161:PRO:HG2	2:B:184:GLY:O	2.21	0.40
2:B:165:ARG:CG	2:B:169:LYS:HE3	2.52	0.40
2:F:61:GLU:CD	2:F:61:GLU:N	2.72	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	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
1	C	40/44 (91%)	36 (90%)	4 (10%)	0	100	100
1	E	40/44 (91%)	34 (85%)	5 (12%)	1 (2%)	5	6
2	B	256/258 (99%)	237 (93%)	15 (6%)	4 (2%)	9	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	256/258 (99%)	225 (88%)	23 (9%)	8 (3%)	4	3
2	F	256/258 (99%)	237 (93%)	16 (6%)	3 (1%)	13	19
All	All	888/906 (98%)	807 (91%)	65 (7%)	16 (2%)	8	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	186(B)	ASP
2	B	186(C)	THR
2	D	97(A)	GLU
2	D	186(B)	ASP
2	D	223	GLY
2	D	224	LYS
2	B	149(A)	THR
2	D	186	VAL
2	F	186	VAL
2	F	186(B)	ASP
2	F	186(C)	THR
2	B	186	VAL
2	D	186(C)	THR
2	D	222	LYS
2	D	186(A)	ASN
1	E	1(J)	GLU

### 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	37/39 (95%)	35 (95%)	2 (5%)	22	36
1	C	37/39 (95%)	37 (100%)	0	100	100
1	E	37/39 (95%)	36 (97%)	1 (3%)	44	65
2	B	227/227 (100%)	216 (95%)	11 (5%)	25	41
2	D	227/227 (100%)	222 (98%)	5 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	227/227 (100%)	219 (96%)	8 (4%)	36	55
All	All	792/798 (99%)	765 (97%)	27 (3%)	37	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(N)	THR
1	A	14(L)	ASP
2	B	21	ASP
2	B	34	PHE
2	B	64	LEU
2	B	73	ARG
2	B	131	ARG
2	B	145	ARG
2	B	157	VAL
2	B	185	LYS
2	B	186	VAL
2	B	186(C)	THR
2	B	204(B)	ASN
2	D	90	VAL
2	D	149(C)	ILE
2	D	157	VAL
2	D	185	LYS
2	D	204(B)	ASN
1	E	1(C)	GLU
2	F	64	LEU
2	F	126	LYS
2	F	129(B)	SER
2	F	147	THR
2	F	157	VAL
2	F	185	LYS
2	F	204(B)	ASN
2	F	221(A)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	71	HIS
2	B	149(B)	ASN
2	B	149(D)	ASN
2	B	204(B)	ASN

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Mol	Chain	Res	Type
2	B	209	GLN
2	D	71	HIS
2	D	78	ASN
2	D	95	ASN
2	D	151	GLN
2	D	204(B)	ASN
2	D	209	GLN
2	F	71	HIS
2	F	149(B)	ASN
2	F	149(D)	ASN
2	F	204(B)	ASN
2	F	209	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](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	F	301	-	4,4,4	0.33	0	6,6,6	0.06	0
4	NAG	F	401	2	14,14,15	1.54	4 (28%)	17,19,21	1.80	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	401	2	14,14,15	1.57	4 (28%)	17,19,21	1.80	4 (23%)
3	SO4	D	302	-	4,4,4	0.30	0	6,6,6	0.05	0
3	SO4	B	307	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	D	306	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	F	305	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	B	303	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	D	304	-	4,4,4	0.30	0	6,6,6	0.09	0
4	NAG	B	401	2	14,14,15	1.56	3 (21%)	17,19,21	1.86	4 (23%)

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	NAG	D	401	2	-	2/6/23/26	0/1/1/1
4	NAG	F	401	2	-	2/6/23/26	0/1/1/1
4	NAG	B	401	2	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	NAG	C3-C2	3.20	1.59	1.52
4	F	401	NAG	C3-C2	2.93	1.58	1.52
4	D	401	NAG	C3-C2	2.80	1.58	1.52
4	B	401	NAG	C4-C5	2.76	1.58	1.53
4	F	401	NAG	C4-C5	2.70	1.58	1.53
4	D	401	NAG	C4-C5	2.65	1.58	1.53
4	D	401	NAG	C4-C3	2.32	1.58	1.52
4	D	401	NAG	O5-C1	2.20	1.47	1.43
4	F	401	NAG	C4-C3	2.17	1.57	1.52
4	F	401	NAG	O5-C1	2.14	1.47	1.43
4	B	401	NAG	C4-C3	2.07	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	NAG	O5-C1-C2	-3.69	105.46	111.29
4	D	401	NAG	C6-C5-C4	3.66	121.58	113.00
4	B	401	NAG	O5-C1-C2	-3.61	105.58	111.29
4	B	401	NAG	C1-C2-N2	-3.55	104.43	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	NAG	C6-C5-C4	3.54	121.29	113.00
4	B	401	NAG	C6-C5-C4	3.51	121.23	113.00
4	D	401	NAG	O5-C1-C2	-3.41	105.90	111.29
4	F	401	NAG	C1-C2-N2	-3.37	104.73	110.49
4	D	401	NAG	C1-C2-N2	-3.34	104.78	110.49
4	B	401	NAG	C1-O5-C5	-2.42	108.91	112.19
4	D	401	NAG	C1-O5-C5	-2.18	109.24	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
4	F	401	NAG	C8-C7-N2-C2
4	F	401	NAG	O7-C7-N2-C2
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	42/44 (95%)	-0.53	0 100 100	33, 43, 60, 78	0
1	C	42/44 (95%)	-0.08	4 (9%) 8 7	40, 56, 77, 99	0
1	E	42/44 (95%)	0.35	3 (7%) 16 14	43, 62, 93, 99	0
2	B	258/258 (100%)	0.22	15 (5%) 23 22	23, 45, 80, 98	0
2	D	258/258 (100%)	0.37	32 (12%) 4 3	26, 51, 94, 99	0
2	F	258/258 (100%)	0.17	15 (5%) 23 22	30, 52, 80, 99	0
All	All	900/906 (99%)	0.20	69 (7%) 13 12	23, 50, 89, 99	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	186(C)	THR	8.9
2	D	186(D)	LYS	6.4
2	F	186(C)	THR	5.6
1	E	14(K)	ILE	5.5
1	E	1(P)	PHE	5.1
1	E	14(L)	ASP	4.8
2	D	221(A)	ARG	4.5
2	D	186(B)	ASP	3.5
2	F	198	PRO	3.4
2	D	222	LYS	3.4
2	B	213	VAL	3.3
2	D	97(A)	GLU	3.3
2	B	198	PRO	3.2
2	D	187	ARG	3.2
2	F	186	VAL	3.2
2	B	186(C)	THR	3.1
2	B	246	GLY	3.1
2	F	53	LEU	3.1
2	F	42	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	14(L)	ASP	3.0
2	F	186(D)	LYS	2.9
2	B	76	TYR	2.9
2	D	221	ASP	2.8
2	F	243	ASP	2.8
2	D	97	ARG	2.8
2	D	198	PRO	2.8
2	F	211	GLY	2.8
1	C	11	SER	2.7
1	C	14(K)	ILE	2.7
2	B	77(A)	ARG	2.7
2	D	60(E)	ASP	2.7
2	D	213	VAL	2.7
2	B	78	ASN	2.7
2	D	175	ARG	2.6
2	B	42	CYS	2.6
2	D	212	ILE	2.6
2	D	170	ALA	2.6
2	F	213	VAL	2.6
2	D	60(C)	PRO	2.5
2	B	212	ILE	2.5
2	D	224	LYS	2.5
2	D	44	ALA	2.5
2	D	211	GLY	2.4
2	F	44	ALA	2.4
2	D	197	GLY	2.4
2	D	185	LYS	2.4
2	B	197	GLY	2.4
2	D	186	VAL	2.4
2	F	212	ILE	2.4
2	D	45	SER	2.3
2	D	174	ILE	2.3
2	B	45	SER	2.3
2	F	197	GLY	2.3
2	F	199	PHE	2.2
2	D	217	ALA	2.2
2	D	186(A)	ASN	2.2
2	D	173	ARG	2.2
2	B	200	VAL	2.2
2	D	31	VAL	2.2
2	B	53	LEU	2.1
2	B	209	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	97	ARG	2.1
2	B	139	THR	2.1
2	D	138	VAL	2.0
2	D	60(D)	TRP	2.0
2	F	45	SER	2.0
2	D	139	THR	2.0
2	D	200	VAL	2.0
1	C	14(D)	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	D	401	14/15	0.65	0.48	88,99,99,99	0
4	NAG	B	401	14/15	0.73	0.29	90,96,99,99	0
4	NAG	F	401	14/15	0.83	0.38	97,99,99,99	0
3	SO4	F	301	5/5	0.90	0.26	97,99,99,99	0
3	SO4	B	307	5/5	0.91	0.27	99,99,99,99	0
3	SO4	D	302	5/5	0.91	0.20	94,95,99,99	0
3	SO4	D	306	5/5	0.93	0.30	99,99,99,99	0
3	SO4	B	303	5/5	0.93	0.28	97,98,99,99	0
3	SO4	F	305	5/5	0.93	0.18	94,97,99,99	0
3	SO4	D	304	5/5	0.95	0.12	94,94,99,99	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.