



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 04:27 AM EDT

PDB ID : 3LU9 / pdb\_00003lu9  
Title : Crystal structure of human thrombin mutant S195A in complex with the extracellular fragment of human PAR1  
Authors : Gandhi, P.S.; Chen, Z.; Di Cera, E.  
Deposited on : 2010-02-17  
Resolution : 1.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

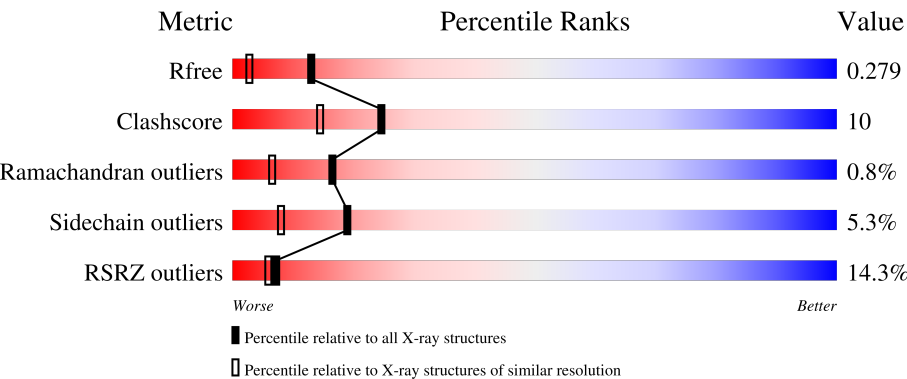
MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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 <sub>free</sub>	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	46	<div><div>9%</div><div>83%</div><div>13%</div><div>.</div></div>
1	D	46	<div><div>13%</div><div>85%</div><div>13%</div><div>.</div></div>
2	B	259	<div><div>5%</div><div>78%</div><div>16%</div><div>..</div></div>
2	E	259	<div><div>16%</div><div>78%</div><div>17%</div><div>..</div></div>
3	C	25	<div><div>52%</div><div>52%</div><div>20%</div><div>12%</div><div>16%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	25	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (56%), green (44%), yellow (40%), and orange (16%). The percentages are labeled above and below the segments.

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5949 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	S	0	0	0
			362	228	58	75	1			
1	D	45	Total	C	N	O	S	0	0	0
			366	230	59	76	1			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	0	0
			2033	1298	360	361	14			
2	E	251	Total	C	N	O	S	0	0	0
			2028	1294	359	361	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	engineered mutation	UNP P00734
E	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 3 is a protein called Proteinase-activated receptor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	0	0	0
			213	136	36	41			
3	F	25	Total	C	N	O	52	0	0
			213	136	36	41			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

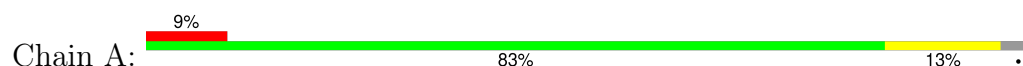
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total	O	0	0
			73	73		
7	B	281	Total	O	0	0
			281	281		
7	C	31	Total	O	0	0
			31	31		
7	D	60	Total	O	0	0
			60	60		
7	E	228	Total	O	0	0
			228	228		
7	F	25	Total	O	0	0
			25	25		

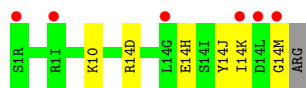
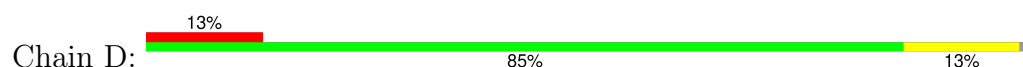
### 3 Residue-property plots [i](#)

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.

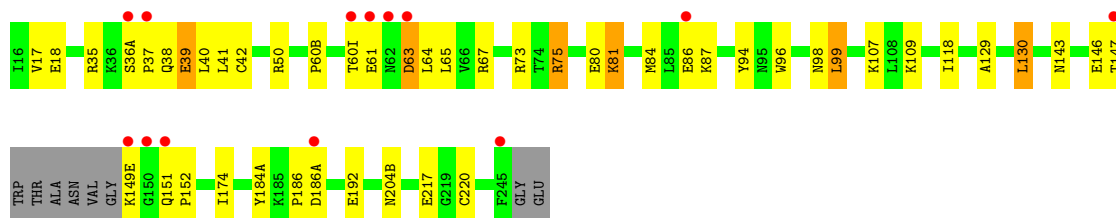
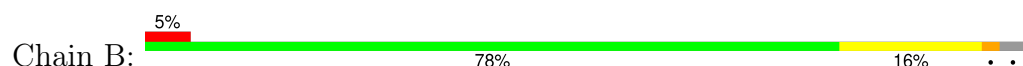
#### • Molecule 1: Prothrombin



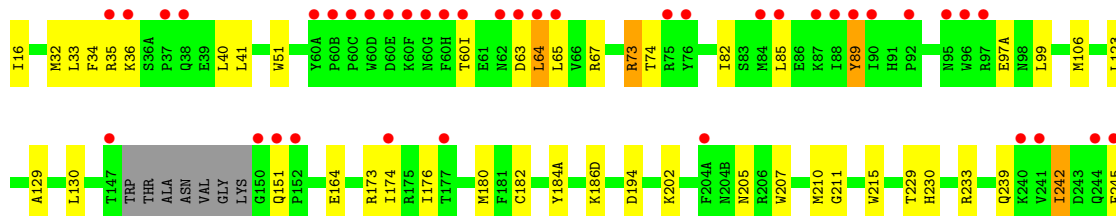
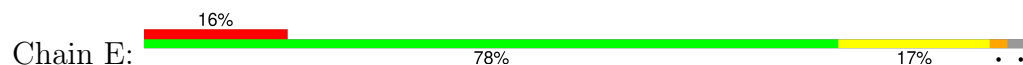
#### • Molecule 1: Prothrombin



#### • Molecule 2: Prothrombin

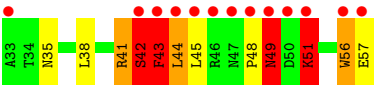


#### • Molecule 2: Prothrombin

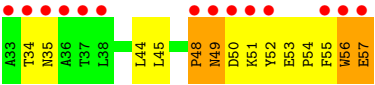




● Molecule 3: Proteinase-activated receptor 1



● Molecule 3: Proteinase-activated receptor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.33Å 50.17Å 85.50Å 76.39° 83.93° 73.74°	Depositor
Resolution (Å)	28.07 – 1.80 28.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.07-1.80) 96.0 (28.07-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.193 , 0.236 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	3162 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% 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: NA, NAG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.78	1/369 (0.3%)	0.73	0/494
1	D	0.68	0/373	0.76	0/499
2	B	0.80	1/2085 (0.0%)	0.86	1/2816 (0.0%)
2	E	0.71	1/2080 (0.0%)	0.86	0/2810
3	C	0.84	0/220	1.76	5/299 (1.7%)
3	F	0.67	0/220	1.07	1/299 (0.3%)
All	All	0.76	3/5347 (0.1%)	0.91	7/7217 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	GLU	C-O	-6.14	1.17	1.24
1	A	1(I)	ARG	NE-CZ	5.52	1.39	1.33
2	E	73	ARG	C-O	-5.10	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	41	ARG	CA-C-N	-11.39	106.94	123.00
3	C	41	ARG	C-N-CA	-11.39	106.94	123.00
3	C	42	SER	N-CA-C	10.85	126.10	108.41
3	C	51	LYS	N-CA-C	10.00	125.10	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60(B)	PRO	N-CA-C	6.43	118.54	110.70
3	F	51	LYS	N-CA-C	5.31	117.69	107.44
3	C	41	ARG	N-CA-C	5.04	119.00	113.21

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	41	ARG	Peptide
3	C	43	PHE	Peptide
3	C	51	LYS	Peptide

## 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	362	0	341	4	0
1	D	366	0	344	5	0
2	B	2033	0	2013	44	0
2	E	2028	0	2003	39	0
3	C	213	0	196	20	0
3	F	213	0	196	16	0
4	B	14	0	13	0	0
4	E	14	0	13	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	6	0	8	0	0
7	A	73	0	0	0	0
7	B	281	0	0	0	0
7	C	31	0	0	3	0
7	D	60	0	0	2	0
7	E	228	0	0	7	0
7	F	25	0	0	1	0
All	All	5949	0	5127	100	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 10.

All (100) 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:39:GLU:OE2	3:C:44:LEU:HB2	1.63	0.99
2:B:75:ARG:HD2	7:C:347:HOH:O	1.65	0.94
2:E:34:PHE:HE1	3:F:52:TYR:CD2	1.94	0.85
2:E:180:MET:HE2	2:E:215:TRP:HE1	1.42	0.84
2:B:143:ASN:HD21	3:C:43:PHE:HE2	1.27	0.80
2:E:73:ARG:HH22	3:F:48:PRO:HD3	1.47	0.79
2:B:41:LEU:HD23	3:C:44:LEU:CD2	2.14	0.77
1:A:1(F):GLY:HA3	2:B:50:ARG:HD2	1.66	0.76
2:E:34:PHE:CE1	3:F:52:TYR:CD2	2.73	0.76
2:B:146:GLU:O	2:B:147:THR:HB	1.90	0.70
2:B:73:ARG:CZ	2:B:151:GLN:HG2	2.25	0.67
2:B:67:ARG:HD2	2:B:80:GLU:OE1	1.95	0.66
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.78	0.66
2:B:73:ARG:HH22	3:C:48:PRO:HD3	1.60	0.66
2:E:74:THR:HG22	3:F:52:TYR:CE1	2.31	0.65
2:B:63:ASP:O	2:B:64:LEU:HD23	1.97	0.65
2:B:192:GLU:HG2	3:C:43:PHE:CE1	2.31	0.65
2:B:41:LEU:HA	3:C:44:LEU:HD23	1.80	0.64
1:A:14(D):ARG:O	1:A:14(H):GLU:HG3	1.97	0.64
2:E:34:PHE:CE1	3:F:52:TYR:HD2	2.15	0.64
2:E:239:GLN:C	7:E:371:HOH:O	2.40	0.64
3:C:48:PRO:O	3:C:49:ASN:HB3	2.00	0.61
2:B:41:LEU:CD1	2:B:64:LEU:HD22	2.32	0.59
2:E:242:ILE:N	7:E:371:HOH:O	2.35	0.59
2:B:143:ASN:ND2	3:C:43:PHE:CE2	2.72	0.58
3:C:42:SER:HB3	7:C:287:HOH:O	2.04	0.58
7:E:418:HOH:O	3:F:54:PRO:HA	2.04	0.57
2:E:85:LEU:HB3	7:E:601:HOH:O	2.05	0.57
2:B:60(I):THR:O	2:B:63:ASP:HB2	2.05	0.56
2:E:184(A):TYR:CE1	2:E:186(D):LYS:HD2	2.41	0.56
7:E:325:HOH:O	3:F:52:TYR:HB2	2.05	0.55
2:B:41:LEU:HD23	3:C:44:LEU:HD23	1.90	0.54
2:B:41:LEU:HD11	2:B:64:LEU:HD22	1.88	0.54
2:E:32:MET:HG3	2:E:40:LEU:HD12	1.88	0.54
2:B:61:GLU:CG	2:B:87:LYS:HA	2.38	0.54
2:B:186:PRO:O	2:B:186(A):ASP:HB2	2.08	0.54
2:E:202:LYS:HE2	2:E:205:ASN:OD1	2.08	0.54
2:E:35:ARG:HB2	2:E:41:LEU:HG	1.90	0.54
2:E:33:LEU:HD11	2:E:64:LEU:HD13	1.90	0.53
2:E:60(I):THR:O	2:E:63:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:THR:HG21	3:F:48:PRO:HG2	1.90	0.53
2:B:40:LEU:O	3:C:44:LEU:HB3	2.08	0.53
2:E:51:TRP:HZ2	2:E:246:GLY:HA2	1.73	0.52
2:B:174:ILE:HG23	3:C:35:ASN:ND2	2.25	0.52
2:B:65:LEU:CD2	2:B:84:MET:SD	2.98	0.52
2:E:34:PHE:HE1	3:F:52:TYR:CE2	2.27	0.52
2:B:42:CYS:SG	3:C:42:SER:HB2	2.50	0.51
3:F:53:GLU:HB3	7:F:564:HOH:O	2.11	0.50
2:E:89:TYR:HB2	7:E:606:HOH:O	2.12	0.50
2:E:67:ARG:HG2	2:E:82:ILE:HG13	1.95	0.49
2:E:97(A):GLU:O	3:F:35:ASN:ND2	2.46	0.49
2:E:41:LEU:CD1	2:E:64:LEU:HD22	2.43	0.49
2:B:42:CYS:SG	3:C:42:SER:CB	3.00	0.48
2:B:35:ARG:HD2	2:B:37:PRO:O	2.14	0.48
2:E:184(A):TYR:CZ	2:E:186(D):LYS:HD2	2.49	0.48
2:E:65:LEU:HD13	3:F:55:PHE:HE2	1.79	0.47
3:C:38:LEU:HD23	3:C:38:LEU:C	2.40	0.47
2:E:36:LYS:HA	7:E:518:HOH:O	2.13	0.47
2:E:130:LEU:HG	2:E:210:MET:HE2	1.97	0.46
2:B:17:VAL:HG12	2:B:18:GLU:HG2	1.97	0.46
2:E:211:GLY:HA2	2:E:229:THR:O	2.16	0.46
2:B:35:ARG:O	2:B:38:GLN:HA	2.16	0.46
1:D:14(K):ILE:C	1:D:14(M):GLY:H	2.23	0.46
2:E:129:ALA:HA	2:E:210:MET:HE1	1.97	0.45
1:A:14(H):GLU:HA	1:A:14(K):ILE:HD12	1.99	0.45
2:B:65:LEU:HD23	2:B:84:MET:SD	2.56	0.45
2:B:65:LEU:HD21	2:B:84:MET:SD	2.57	0.45
2:B:86:GLU:OE2	2:B:107:LYS:HE3	2.17	0.45
2:B:80:GLU:C	2:B:81:LYS:HD2	2.43	0.44
2:B:81:LYS:HD3	2:B:118:ILE:HD12	2.00	0.44
2:E:202:LYS:CE	2:E:205:ASN:OD1	2.66	0.43
3:F:56:TRP:HB3	3:F:57:GLU:H	1.70	0.43
1:D:14(J):TYR:O	7:D:390:HOH:O	2.21	0.43
2:B:41:LEU:O	3:C:42:SER:OG	2.35	0.43
2:E:85:LEU:HD22	2:E:106:MET:HB3	2.00	0.43
2:E:89:TYR:HE1	2:E:245:PHE:CE1	2.37	0.43
1:A:1(Q):GLU:HB3	2:B:204(B):ASN:HB2	2.01	0.43
2:E:73:ARG:NH1	3:F:52:TYR:OH	2.50	0.43
2:B:98:ASN:O	2:B:99:LEU:HB2	2.17	0.43
2:B:129:ALA:O	2:B:130:LEU:HB2	2.18	0.42
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184(A):TYR:HE1	2:E:173:ARG:NH2	2.16	0.42
2:B:36(A):SER:HA	2:B:37:PRO:HA	1.92	0.42
1:D:10:LYS:NZ	7:D:138:HOH:O	2.40	0.42
1:D:14(D):ARG:O	1:D:14(H):GLU:HG3	2.19	0.42
1:D:14(K):ILE:C	1:D:14(M):GLY:N	2.77	0.42
3:F:34:THR:O	3:F:34:THR:HG23	2.20	0.42
2:B:174:ILE:HG23	3:C:35:ASN:HD22	1.84	0.42
2:B:151:GLN:HG3	2:B:152:PRO:HD2	2.01	0.42
3:C:48:PRO:O	3:C:49:ASN:CB	2.67	0.42
2:E:74:THR:HG21	3:F:48:PRO:CG	2.50	0.41
3:C:44:LEU:O	3:C:45:LEU:HB2	2.18	0.41
2:E:202:LYS:HD2	2:E:207:TRP:CE2	2.56	0.41
2:E:16:ILE:N	2:E:194:ASP:OD2	2.54	0.41
2:B:35:ARG:HE	2:B:41:LEU:HD21	1.86	0.41
2:E:230:HIS:CG	2:E:233:ARG:HG3	2.56	0.41
2:B:192:GLU:OE1	2:B:220:CYS:SG	2.79	0.40
2:E:89:TYR:CE1	2:E:245:PHE:HE1	2.39	0.40
3:C:35:ASN:HB2	7:C:623:HOH:O	2.20	0.40
2:E:89:TYR:CE1	2:E:245:PHE:CE1	3.09	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	42/46 (91%)	39 (93%)	3 (7%)	0	100	100
1	D	43/46 (94%)	40 (93%)	3 (7%)	0	100	100
2	B	247/259 (95%)	237 (96%)	10 (4%)	0	100	100
2	E	247/259 (95%)	237 (96%)	10 (4%)	0	100	100
3	C	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	23/25 (92%)	15 (65%)	5 (22%)	3 (13%)	0	0
All	All	625/660 (95%)	587 (94%)	33 (5%)	5 (1%)	16	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	49	ASN
3	F	49	ASN
3	C	56	TRP
3	F	45	LEU
3	F	48	PRO

### 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	40/41 (98%)	40 (100%)	0	100	100
1	D	40/41 (98%)	40 (100%)	0	100	100
2	B	219/224 (98%)	211 (96%)	8 (4%)	29	17
2	E	218/224 (97%)	208 (95%)	10 (5%)	23	11
3	C	23/23 (100%)	16 (70%)	7 (30%)	0	0
3	F	23/23 (100%)	18 (78%)	5 (22%)	1	0
All	All	563/576 (98%)	533 (95%)	30 (5%)	19	8

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	39	GLU
2	B	63	ASP
2	B	75	ARG
2	B	81	LYS
2	B	99	LEU
2	B	109	LYS

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Mol	Chain	Res	Type
2	B	130	LEU
2	B	149(E)	LYS
3	C	42	SER
3	C	43	PHE
3	C	44	LEU
3	C	49	ASN
3	C	51	LYS
3	C	56	TRP
3	C	57	GLU
2	E	64	LEU
2	E	89	TYR
2	E	99	LEU
2	E	123	LEU
2	E	151	GLN
2	E	164	GLU
2	E	174	ILE
2	E	176	ILE
2	E	182	CYS
2	E	242	ILE
3	F	44	LEU
3	F	49	ASN
3	F	50	ASP
3	F	56	TRP
3	F	57	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	62	ASN
2	B	131	GLN
2	B	151	GLN
2	B	179	ASN
2	B	204(B)	ASN
2	B	209	GLN
2	E	71	HIS
2	E	131	GLN
2	E	151	GLN
2	E	204(B)	ASN
2	E	209	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	NAG	E	400	2	14,14,15	0.43	0	17,19,21	1.31	2 (11%)
6	GOL	B	402	-	5,5,5	0.45	0	5,5,5	0.68	0
4	NAG	B	400	2	14,14,15	0.48	0	17,19,21	1.73	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	E	400	2	-	2/6/23/26	0/1/1/1
6	GOL	B	402	-	-	2/4/4/4	-
4	NAG	B	400	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	NAG	C1-O5-C5	4.61	118.37	112.19
4	E	400	NAG	C1-O5-C5	3.13	116.38	112.19
4	E	400	NAG	O5-C1-C2	-2.36	107.64	111.29
4	B	400	NAG	C6-C5-C4	-2.36	107.24	113.02
4	B	400	NAG	O5-C1-C2	-2.23	107.85	111.29
4	B	400	NAG	C8-C7-N2	2.16	119.70	116.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	400	NAG	C8-C7-N2-C2
4	B	400	NAG	O7-C7-N2-C2
4	E	400	NAG	C8-C7-N2-C2
4	E	400	NAG	O7-C7-N2-C2
6	B	402	GOL	C1-C2-C3-O3
6	B	402	GOL	O2-C2-C3-O3
4	B	400	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	44/46 (95%)	0.52	4 (9%) 16 14	14, 24, 45, 54	0
1	D	45/46 (97%)	0.93	6 (13%) 8 6	14, 33, 59, 66	0
2	B	251/259 (96%)	0.21	13 (5%) 34 31	8, 23, 47, 65	0
2	E	251/259 (96%)	0.81	41 (16%) 5 4	11, 34, 74, 90	0
3	C	25/25 (100%)	2.46	13 (52%) 0 0	16, 38, 94, 114	0
3	F	19/25 (76%)	2.97	14 (73%) 0 0	25, 60, 100, 104	0
All	All	635/660 (96%)	0.69	91 (14%) 7 6	8, 28, 72, 114	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14(M)	GLY	7.2
3	C	45	LEU	6.9
3	F	48	PRO	6.7
3	C	42	SER	6.3
2	B	147	THR	5.9
2	E	89	TYR	5.5
3	F	56	TRP	5.5
1	A	1(R)	SER	5.5
3	C	44	LEU	5.4
3	C	56	TRP	5.3
2	E	152	PRO	5.2
2	E	245	PHE	4.7
3	F	34	THR	4.7
1	A	14(L)	ASP	4.7
2	E	147	THR	4.6
2	E	38	GLN	4.5
2	E	150	GLY	4.4
1	D	14(K)	ILE	4.4
1	D	14(L)	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	245	PHE	4.2
2	E	92	PRO	4.2
2	E	60(F)	LYS	4.2
3	C	50	ASP	4.1
3	F	50	ASP	4.1
1	D	14(G)	LEU	4.1
2	E	151	GLN	4.1
3	C	47	ASN	4.1
3	F	36	ALA	4.0
2	B	149(E)	LYS	4.0
3	F	33	ALA	4.0
3	C	43	PHE	4.0
2	B	60(I)	THR	4.0
2	B	150	GLY	4.0
2	E	37	PRO	4.0
2	E	64	LEU	3.8
2	E	85	LEU	3.8
3	F	49	ASN	3.6
3	F	35	ASN	3.6
3	C	48	PRO	3.5
1	A	14(K)	ILE	3.3
2	E	246	GLY	3.3
2	E	60(D)	TRP	3.2
2	E	88	ILE	3.2
3	F	51	LYS	3.1
2	E	60(H)	PHE	3.1
2	B	37	PRO	3.1
2	E	84	MET	3.1
2	E	96	TRP	3.0
3	F	55	PHE	3.0
3	C	46	ARG	2.9
3	F	52	TYR	2.9
3	C	49	ASN	2.9
3	C	33	ALA	2.8
2	E	60(B)	PRO	2.7
2	E	36	LYS	2.6
2	B	62	ASN	2.6
1	D	1(R)	SER	2.6
1	A	1(Q)	GLU	2.6
2	E	75	ARG	2.5
2	E	65	LEU	2.5
2	E	60(I)	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	36(A)	SER	2.4
2	E	97	ARG	2.4
2	B	151	GLN	2.4
2	E	90	ILE	2.4
2	E	60(C)	PRO	2.4
2	E	204(A)	PHE	2.4
3	C	57	GLU	2.4
2	E	60(A)	TYR	2.3
2	E	63	ASP	2.3
3	F	37	THR	2.3
2	B	186(A)	ASP	2.3
2	E	244	GLN	2.3
3	C	51	LYS	2.3
2	E	76	TYR	2.2
2	B	86	GLU	2.2
2	E	241	VAL	2.2
2	E	62	ASN	2.2
2	E	174	ILE	2.2
3	F	57	GLU	2.2
1	D	1(I)	ARG	2.2
2	E	240	LYS	2.2
3	F	38	LEU	2.2
2	B	61	GLU	2.1
2	E	35	ARG	2.1
2	E	177	THR	2.1
2	E	87	LYS	2.1
2	E	60(G)	ASN	2.1
2	E	95	ASN	2.0
2	B	63	ASP	2.0
2	E	60(E)	ASP	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 [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, 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	E	400	14/15	0.48	0.17	52,58,62,63	0
4	NAG	B	400	14/15	0.66	0.15	45,52,54,55	0
6	GOL	B	402	6/6	0.87	0.12	27,36,38,39	0
5	NA	E	401	1/1	0.97	0.15	27,27,27,27	0
5	NA	B	401	1/1	0.98	0.08	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.