



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:11 PM GMT

PDB ID : 1SG8
Title : Crystal structure of the procoagulant fast form of thrombin
Authors : Pineda, A.O.; Carrell, C.J.; Bush, L.A.; Prasad, S.; Caccia, S.; Chen, Z.W.;
Mathews, F.S.; Di Cera, E.
Deposited on : 2004-02-23
Resolution : 2.30 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

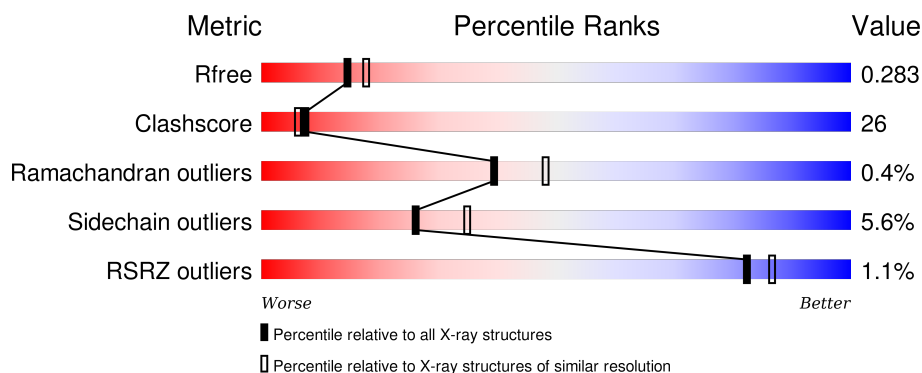
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	36	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>17%</div> <div>6%</div> <div>25%</div> </div> </div>
1	D	36	<div> <div></div> <div> <div>47%</div> <div>25%</div> <div>•</div> <div>25%</div> </div> </div>
2	B	259	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>• •</div> </div> </div>
2	E	259	<div> <div></div> <div> <div>55%</div> <div>39%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4864 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			
1	D	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	0	0
			2021	1294	351	362	14			
2	E	251	Total	C	N	O	S	0	0	0
			2024	1292	356	362	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77A	ALA	ARG	ENGINEERED	UNP P00734
E	77A	ALA	ARG	ENGINEERED	UNP P00734

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	174	Total	O	0	0
			174	174		
5	D	7	Total	O	0	0
			7	7		
5	E	146	Total	O	0	0
			146	146		

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.

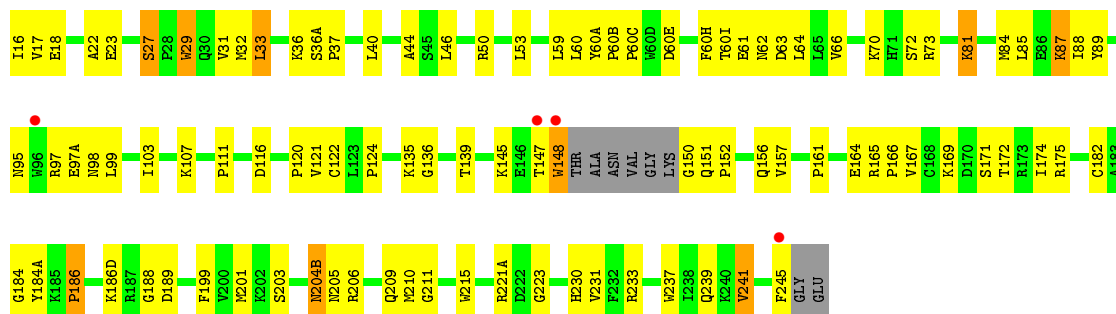
• Molecule 1: thrombin



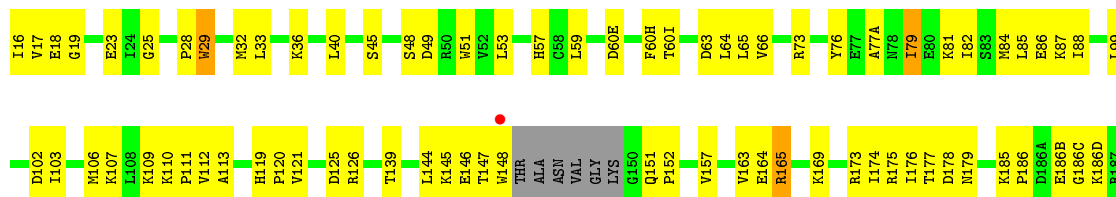
• Molecule 1: thrombin



• Molecule 2: thrombin



• Molecule 2: thrombin



G188	D189	A190	S195	G196	G197	P198	F199	V200	M201	K202	S203	P204	F204A	N204B	N205	R206	M210	G211	I212	V213	S214	M215	C220	D222	G223	K224	F227	Y228	T229	R230	V231	F232	R233	R240	V241	I242	D243	Q244	F245	GLY	GLU
------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.49 Å 65.58 Å 162.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 – 2.30 81.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.7 (24.64-2.30) 79.3 (81.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.20 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.289 0.215 , 0.283	Depositor DCC
R_{free} test set	1724 reflections (7.02%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 29142 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: NA, NAG

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	0.40	0/224	0.71	0/298
1	D	0.51	0/224	0.83	0/298
2	B	0.36	0/2075	0.62	0/2808
2	E	0.39	0/2076	0.67	1/2806 (0.0%)
All	All	0.38	0/4599	0.66	1/6210 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	199	PHE	N-CA-C	-5.35	96.55	111.00

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	222	0	225	11	0
1	D	222	0	225	6	0
2	B	2021	0	1980	94	0
2	E	2024	0	1994	124	0
3	B	14	0	13	3	0
3	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	18	0	0	0	0
5	B	174	0	0	21	1
5	D	7	0	0	0	0
5	E	146	0	0	35	1
All	All	4864	0	4450	230	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (230) 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:184(A):TYR:HB2	5:B:790:HOH:O	1.49	1.09
2:B:84:MET:HG2	5:B:576:HOH:O	1.58	1.03
2:E:84:MET:HG2	5:E:859:HOH:O	1.57	1.03
2:E:177:THR:HG22	2:E:179:ASN:H	1.23	1.00
2:B:239:GLN:HG2	5:B:565:HOH:O	1.61	1.00
2:E:245:PHE:CE2	5:E:835:HOH:O	2.20	0.94
2:E:65:LEU:HD21	5:E:859:HOH:O	1.67	0.93
2:B:145:LYS:HB3	5:B:779:HOH:O	1.67	0.93
2:E:79:ILE:HD12	5:E:685:HOH:O	1.69	0.91
2:E:77(A):ALA:O	5:E:815:HOH:O	1.89	0.90
2:E:45:SER:HB3	2:E:198:PRO:HG3	1.55	0.88
1:A:1:CYS:O	2:B:122:CYS:SG	2.32	0.87
3:B:400:NAG:O6	5:B:904:HOH:O	1.87	0.87
2:B:50:ARG:NH1	2:B:111:PRO:HB3	1.88	0.87
2:E:65:LEU:CD2	5:E:859:HOH:O	2.23	0.85
2:B:174:ILE:O	5:B:747:HOH:O	1.94	0.84
2:E:185:LYS:HG3	5:E:804:HOH:O	1.76	0.83
2:B:165:ARG:HD3	5:B:558:HOH:O	1.79	0.82
1:A:1:CYS:C	2:B:122:CYS:SG	2.57	0.82
2:B:145:LYS:HZ3	2:B:150:GLY:N	1.77	0.82
2:E:73:ARG:HH22	2:E:151:GLN:HB3	1.45	0.81
2:B:139:THR:HG22	2:B:157:VAL:HG22	1.60	0.81
2:E:73:ARG:NH2	2:E:151:GLN:HB3	1.95	0.81
2:E:126:ARG:HD2	5:E:882:HOH:O	1.82	0.80
2:B:81:LYS:NZ	2:B:81:LYS:HB3	1.97	0.80
2:E:165:ARG:NH1	5:E:818:HOH:O	2.14	0.79
2:E:233:ARG:HD2	5:E:671:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:ARG:NH1	2:E:151:GLN:HB3	1.98	0.77
2:E:73:ARG:HH12	2:E:151:GLN:CB	1.96	0.77
2:B:50:ARG:HH12	2:B:111:PRO:HB3	1.49	0.76
2:E:245:PHE:HE2	5:E:835:HOH:O	1.58	0.75
3:B:400:NAG:C6	5:B:904:HOH:O	2.31	0.75
2:E:185:LYS:O	5:E:656:HOH:O	2.03	0.74
2:E:73:ARG:HH12	2:E:151:GLN:HB3	1.50	0.74
2:B:167:VAL:O	2:B:171:SER:HB3	1.88	0.74
2:B:81:LYS:HZ2	2:B:81:LYS:HB3	1.52	0.73
2:E:73:ARG:HH22	2:E:151:GLN:HE21	1.35	0.72
2:E:73:ARG:HH22	2:E:151:GLN:NE2	1.88	0.72
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.71	0.72
2:E:73:ARG:CZ	2:E:151:GLN:HB3	2.20	0.71
2:B:22:ALA:HB2	2:B:157:VAL:HG23	1.71	0.71
2:E:175:ARG:NH2	5:E:574:HOH:O	2.23	0.71
2:E:139:THR:HG22	2:E:157:VAL:HG12	1.71	0.71
2:E:79:ILE:HG13	5:E:815:HOH:O	1.91	0.70
2:B:164:GLU:HB2	2:B:166:PRO:HD2	1.73	0.70
2:E:126:ARG:CD	5:E:882:HOH:O	2.40	0.69
2:B:60(B):PRO:HG2	2:B:60(C):PRO:HD3	1.75	0.69
2:E:76:TYR:O	5:E:690:HOH:O	2.10	0.68
2:B:27:SER:OG	5:B:533:HOH:O	2.06	0.68
2:E:164:GLU:H	2:E:164:GLU:CD	1.96	0.68
2:B:156:GLN:HB2	5:B:548:HOH:O	1.94	0.68
2:B:186:PRO:HG3	2:B:223:GLY:H	1.59	0.67
2:B:36:LYS:HD2	2:B:62:ASN:O	1.94	0.67
2:E:146:GLU:HB2	2:E:220:CYS:HB2	1.78	0.66
2:E:126:ARG:HG3	5:E:681:HOH:O	1.96	0.65
1:A:14(D):ARG:HH11	1:A:14(D):ARG:HG2	1.61	0.65
1:A:14(D):ARG:NH1	1:A:14(D):ARG:HG2	2.11	0.65
2:B:87:LYS:HD3	2:B:88:ILE:N	2.12	0.65
1:D:14(D):ARG:CZ	1:D:14(D):ARG:HB3	2.27	0.64
2:B:33:LEU:HD21	2:B:64:LEU:HD13	1.78	0.64
2:B:237:TRP:O	2:B:241:VAL:HG12	1.97	0.64
2:B:174:ILE:HD12	2:B:215:TRP:CZ3	2.33	0.63
2:E:32:MET:HE3	2:E:40:LEU:HD12	1.81	0.61
2:E:53:LEU:HD11	2:E:103:ILE:HD11	1.82	0.61
2:B:32:MET:HE3	2:B:40:LEU:HD12	1.82	0.61
2:E:25:GLY:O	2:E:28:PRO:HD3	2.01	0.60
2:E:16:ILE:N	5:E:813:HOH:O	2.33	0.60
2:E:173:ARG:N	5:E:557:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14(I):SER:HB3	2:B:135:LYS:HG3	1.83	0.60
2:B:84:MET:CG	5:B:576:HOH:O	2.30	0.60
2:E:202:LYS:HE2	2:E:205:ASN:HB2	1.83	0.60
2:E:79:ILE:CD1	5:E:815:HOH:O	2.50	0.59
2:E:201:MET:HB2	2:E:210:MET:CE	2.30	0.59
2:E:110:LYS:O	5:E:694:HOH:O	2.16	0.59
2:E:245:PHE:CZ	5:E:835:HOH:O	2.45	0.59
2:B:147:THR:HG22	2:B:148:TRP:H	1.67	0.59
1:A:14(A):LYS:HB2	5:B:596:HOH:O	2.03	0.59
2:E:240:LYS:O	2:E:244:GLN:HB3	2.04	0.58
2:E:84:MET:CB	2:E:109:LYS:HD2	2.34	0.58
2:B:221(A):ARG:HG3	5:B:537:HOH:O	2.03	0.58
2:B:87:LYS:HD3	2:B:88:ILE:H	1.67	0.57
2:E:76:TYR:CE2	2:E:77(A):ALA:HB2	2.39	0.57
2:E:139:THR:CG2	2:E:157:VAL:HG12	2.35	0.57
2:B:60(I):THR:OG1	5:B:515:HOH:O	2.17	0.56
2:E:204(B):ASN:C	2:E:204(B):ASN:HD22	2.08	0.56
2:B:73:ARG:HD3	2:B:152:PRO:O	2.04	0.56
2:E:177:THR:HG22	2:E:178:ASP:N	2.19	0.56
2:E:79:ILE:CD1	5:E:685:HOH:O	2.40	0.56
2:B:40:LEU:C	2:B:40:LEU:HD23	2.24	0.56
2:B:147:THR:HG22	2:B:148:TRP:N	2.20	0.56
2:E:57:HIS:CE1	2:E:195:SER:HB3	2.41	0.56
2:E:144:LEU:HG	2:E:152:PRO:HG3	1.87	0.56
2:E:59:LEU:HD21	2:E:106:MET:HE3	1.88	0.56
2:E:79:ILE:CG1	5:E:815:HOH:O	2.52	0.56
3:B:400:NAG:H61	5:B:904:HOH:O	1.99	0.56
2:E:66:VAL:HG23	2:E:85:LEU:HD21	1.87	0.56
1:A:14(D):ARG:CG	1:A:14(D):ARG:HH11	2.19	0.55
2:B:22:ALA:HB2	2:B:157:VAL:CG2	2.37	0.55
2:E:222:ASP:HA	5:E:651:HOH:O	2.05	0.55
2:B:186:PRO:HG3	2:B:223:GLY:N	2.21	0.55
2:E:16:ILE:HG12	5:E:813:HOH:O	2.06	0.54
2:E:177:THR:CG2	2:E:178:ASP:N	2.70	0.54
1:D:5:PRO:HA	1:D:9:LYS:HB2	1.88	0.54
2:E:76:TYR:C	5:E:690:HOH:O	2.46	0.54
2:B:169:LYS:HB3	2:B:169:LYS:NZ	2.22	0.54
1:A:6:LEU:CD2	2:B:116:ASP:HB3	2.39	0.53
2:E:175:ARG:NH1	5:E:583:HOH:O	2.40	0.53
2:E:63:ASP:HB3	5:E:680:HOH:O	2.08	0.53
2:E:211:GLY:HA2	2:E:231:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ASN:ND2	5:B:791:HOH:O	2.42	0.53
2:E:178:ASP:HB2	2:E:233:ARG:NH1	2.24	0.52
1:A:6:LEU:HD22	2:B:116:ASP:HB3	1.92	0.52
2:E:185:LYS:HB3	2:E:186:PRO:HD2	1.89	0.52
2:B:53:LEU:HD11	2:B:103:ILE:HD11	1.90	0.52
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.07	0.52
2:E:79:ILE:HD12	5:E:815:HOH:O	2.10	0.52
2:B:188:GLY:O	2:B:189:ASP:HB2	2.10	0.52
2:E:147:THR:O	2:E:148:TRP:CB	2.57	0.52
2:E:189:ASP:HB2	5:E:652:HOH:O	2.09	0.52
2:B:31:VAL:HB	2:B:44:ALA:HB3	1.92	0.52
1:D:14(J):TYR:O	1:D:14(K):ILE:HB	2.09	0.52
2:E:73:ARG:HH22	2:E:151:GLN:CB	2.19	0.51
2:B:87:LYS:HB3	2:B:89:TYR:CE2	2.46	0.51
2:E:33:LEU:HD21	2:E:64:LEU:HD13	1.94	0.50
2:E:99:LEU:HD12	2:E:215:TRP:HB3	1.92	0.50
2:E:73:ARG:HH12	2:E:151:GLN:CG	2.25	0.50
2:E:203:SER:O	2:E:205:ASN:HA	2.12	0.50
2:B:204(B):ASN:O	2:B:205:ASN:HB2	2.11	0.50
2:B:184(A):TYR:CB	5:B:790:HOH:O	2.28	0.50
2:B:17:VAL:HG12	2:B:18:GLU:HG2	1.94	0.50
2:E:144:LEU:CD2	2:E:152:PRO:HG3	2.42	0.49
2:E:84:MET:HB2	2:E:109:LYS:HD2	1.94	0.49
2:E:145:LYS:HD2	5:E:635:HOH:O	2.11	0.49
2:E:202:LYS:HE3	2:E:205:ASN:O	2.13	0.49
2:B:29:TRP:CG	2:B:121:VAL:HB	2.49	0.48
2:B:60(B):PRO:CG	2:B:60(C):PRO:HD3	2.43	0.48
1:A:14(H):GLU:O	1:A:14(K):ILE:HG12	2.13	0.48
2:E:82:ILE:N	2:E:82:ILE:HD12	2.29	0.48
2:B:135:LYS:HE2	2:B:184(A):TYR:OH	2.13	0.47
2:B:203:SER:HB3	2:B:204(B):ASN:ND2	2.29	0.47
2:E:73:ARG:NH2	2:E:151:GLN:NE2	2.61	0.47
2:E:144:LEU:CG	2:E:152:PRO:HG3	2.43	0.47
2:B:66:VAL:HG23	2:B:85:LEU:HD21	1.95	0.47
1:D:14(A):LYS:HG2	2:E:23:GLU:CD	2.34	0.47
2:E:60(H):PHE:CG	2:E:64:LEU:HD21	2.49	0.47
2:B:46:LEU:CD1	2:B:120:PRO:HB3	2.45	0.47
2:E:244:GLN:O	2:E:245:PHE:HB2	2.14	0.47
2:E:144:LEU:HD21	2:E:152:PRO:HG3	1.96	0.47
2:B:203:SER:HB3	2:B:204(B):ASN:HD21	1.80	0.47
2:E:212:ILE:HB	2:E:229:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ILE:HD12	2:E:215:TRP:CZ3	2.50	0.47
2:B:59:LEU:HD13	2:B:88:ILE:CG2	2.44	0.47
2:B:50:ARG:HD2	2:B:107:LYS:NZ	2.29	0.47
2:B:161:PRO:HG2	2:B:184:GLY:O	2.14	0.47
2:E:186(C):GLY:N	5:E:838:HOH:O	2.47	0.46
2:E:178:ASP:CB	2:E:233:ARG:NH1	2.78	0.46
2:B:230:HIS:CG	2:B:233:ARG:HG3	2.50	0.46
2:E:163:VAL:HG13	2:E:164:GLU:OE2	2.15	0.46
1:D:14:ASP:HB2	2:E:23:GLU:OE1	2.16	0.46
2:B:98:ASN:O	2:B:99:LEU:HB2	2.15	0.45
2:E:119:HIS:ND1	2:E:120:PRO:HD2	2.31	0.45
2:E:84:MET:HB3	2:E:109:LYS:HD2	1.97	0.45
2:E:107:LYS:NZ	2:E:245:PHE:CE2	2.84	0.45
2:E:177:THR:HG22	2:E:179:ASN:N	2.08	0.45
2:B:89:TYR:HH	2:B:245:PHE:HD2	1.61	0.45
2:E:176:ILE:HD12	2:E:227:PHE:CE2	2.52	0.45
2:B:186(D):LYS:HE2	5:B:590:HOH:O	2.16	0.45
2:E:17:VAL:HG12	2:E:18:GLU:HG2	1.99	0.45
2:B:61:GLU:CD	2:B:61:GLU:H	2.20	0.45
2:B:201:MET:HB2	2:B:210:MET:CE	2.47	0.44
2:B:186(D):LYS:CE	5:B:590:HOH:O	2.66	0.44
2:E:164:GLU:OE2	2:E:185:LYS:NZ	2.51	0.44
2:E:32:MET:HE3	2:E:40:LEU:CD1	2.45	0.44
2:B:148:TRP:C	2:B:148:TRP:CD1	2.91	0.44
2:E:99:LEU:O	2:E:102:ASP:HB2	2.18	0.44
2:E:241:VAL:O	2:E:245:PHE:N	2.51	0.43
2:E:189:ASP:OD1	2:E:190:ALA:N	2.50	0.43
2:B:60(B):PRO:C	2:B:60(E):ASP:H	2.22	0.43
2:B:95:ASN:O	2:B:99:LEU:N	2.51	0.43
2:E:36:LYS:NZ	5:E:831:HOH:O	2.51	0.43
2:B:60(I):THR:O	2:B:61:GLU:C	2.56	0.43
2:E:17:VAL:O	2:E:188:GLY:HA2	2.18	0.43
1:A:14:ASP:HB2	2:B:23:GLU:OE1	2.19	0.43
2:E:66:VAL:CG2	2:E:85:LEU:HD21	2.48	0.43
2:E:49:ASP:OD2	2:E:111:PRO:HB3	2.19	0.43
2:E:29:TRP:CG	2:E:121:VAL:HB	2.53	0.43
2:E:125:ASP:OD2	2:E:125:ASP:N	2.51	0.43
2:B:59:LEU:HD13	2:B:88:ILE:HG23	2.00	0.43
2:E:48:SER:HB3	2:E:51:TRP:HB2	1.99	0.43
2:E:188:GLY:O	2:E:189:ASP:HB2	2.19	0.43
2:B:84:MET:CB	5:B:576:HOH:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:ARG:NH2	2:B:151:GLN:NE2	2.67	0.42
2:E:185:LYS:HB2	2:E:186(B):GLU:HG3	2.01	0.42
2:B:165:ARG:N	2:B:166:PRO:CD	2.82	0.42
2:E:197:GLY:HA2	2:E:198:PRO:HD3	1.80	0.42
2:E:151:GLN:HA	2:E:152:PRO:HD3	1.84	0.42
2:E:19:GLY:N	5:E:816:HOH:O	2.27	0.42
2:E:81:LYS:HD3	2:E:82:ILE:N	2.34	0.42
2:B:60(H):PHE:CG	2:B:64:LEU:HD21	2.53	0.42
2:E:81:LYS:HD3	2:E:82:ILE:H	1.85	0.42
2:E:186(C):GLY:O	2:E:186(D):LYS:HG3	2.20	0.42
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HB2	2.55	0.42
2:B:16:ILE:HB	2:B:156:GLN:HB3	2.02	0.41
2:E:204(B):ASN:HD22	2:E:205:ASN:N	2.19	0.41
2:B:95:ASN:HD21	2:B:97(A):GLU:HB3	1.85	0.41
2:B:97:ARG:HG2	2:B:97:ARG:NH1	2.35	0.41
2:E:204(B):ASN:ND2	2:E:206:ARG:H	2.18	0.41
2:E:178:ASP:CB	2:E:233:ARG:HH11	2.32	0.41
2:B:184:GLY:HA3	5:B:913:HOH:O	2.21	0.41
2:E:203:SER:HA	2:E:204:PRO:HD3	1.73	0.41
2:B:70:LYS:HE3	2:B:72:SER:O	2.21	0.41
2:E:201:MET:HB2	2:E:210:MET:HE2	2.01	0.41
2:E:197:GLY:O	2:E:213:VAL:HG23	2.21	0.41
2:B:60:LEU:HD12	2:B:60(A):TYR:N	2.36	0.41
2:E:99:LEU:CD1	2:E:215:TRP:HB3	2.51	0.41
2:B:97(A):GLU:OE2	2:B:175:ARG:HB3	2.21	0.41
2:E:112:VAL:HG12	2:E:113:ALA:N	2.36	0.41
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.23	0.41
2:B:95:ASN:O	2:B:99:LEU:HA	2.20	0.41
2:B:124:PRO:HD3	2:B:209:GLN:O	2.21	0.41
1:D:4:ARG:HB2	1:D:7:PHE:HB2	2.02	0.40
2:E:87:LYS:CD	2:E:88:ILE:H	2.34	0.40
2:B:36(A):SER:HA	2:B:37:PRO:HA	1.85	0.40
2:E:230:HIS:CG	2:E:233:ARG:HG3	2.56	0.40
2:E:244:GLN:O	2:E:245:PHE:CB	2.69	0.40
2:B:31:VAL:CG1	2:B:66:VAL:HG13	2.50	0.40
2:B:164:GLU:CD	2:B:164:GLU:H	2.25	0.40
2:B:136:GLY:HA3	2:B:199:PHE:CE1	2.57	0.40
2:B:32:MET:HE2	2:B:40:LEU:HG	2.03	0.40
2:E:82:ILE:N	2:E:82:ILE:CD1	2.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:768:HOH:O	5:E:509:HOH:O[3_545]	1.87	0.33

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	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
1	D	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
2	B	247/259 (95%)	222 (90%)	24 (10%)	1 (0%)	39	48
2	E	247/259 (95%)	228 (92%)	18 (7%)	1 (0%)	39	48
All	All	544/590 (92%)	498 (92%)	44 (8%)	2 (0%)	39	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	79	ILE
2	B	186	PRO

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	25/31 (81%)	23 (92%)	2 (8%)	15	18
1	D	25/31 (81%)	23 (92%)	2 (8%)	15	18
2	B	217/224 (97%)	206 (95%)	11 (5%)	29	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	218/224 (97%)	206 (94%)	12 (6%)	27	36
All	All	485/510 (95%)	458 (94%)	27 (6%)	26	35

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

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14(D)	ARG
2	B	27	SER
2	B	29	TRP
2	B	33	LEU
2	B	63	ASP
2	B	81	LYS
2	B	87	LYS
2	B	148	TRP
2	B	172	THR
2	B	182	CYS
2	B	204(B)	ASN
2	B	241	VAL
1	D	6	LEU
1	D	14(D)	ARG
2	E	29	TRP
2	E	60(E)	ASP
2	E	60(I)	THR
2	E	86	GLU
2	E	165	ARG
2	E	169	LYS
2	E	204(B)	ASN
2	E	205	ASN
2	E	210	MET
2	E	224	LYS
2	E	240	LYS
2	E	243	ASP

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

Mol	Chain	Res	Type
2	B	30	GLN
2	B	71	HIS
2	B	151	GLN
2	B	204(B)	ASN

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Mol	Chain	Res	Type
2	E	30	GLN
2	E	71	HIS
2	E	151	GLN
2	E	179	ASN
2	E	204(B)	ASN
2	E	205	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	NAG	B	400	2	14,14,15	0.80	0	15,19,21	2.38	3 (20%)
3	NAG	E	500	2	14,14,15	0.79	0	15,19,21	2.38	3 (20%)

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	B	400	2	-	0/6/23/26	0/1/1/1
3	NAG	E	500	2	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
3	B	400	NAG	C2-N2-C7	-5.80	115.58	123.04
3	E	500	NAG	C2-N2-C7	-5.79	115.60	123.04
3	E	500	NAG	O3-C3-C4	-5.68	97.56	110.34
3	B	400	NAG	O3-C3-C4	-5.66	97.59	110.34
3	B	400	NAG	O7-C7-C8	2.16	126.03	122.06
3	E	500	NAG	O7-C7-C8	2.18	126.06	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	27/36 (75%)	0.00	1 (3%) 45 54	34, 49, 62, 64	0
1	D	27/36 (75%)	-0.07	0 100 100	38, 52, 68, 74	0
2	B	251/259 (96%)	-0.12	4 (1%) 74 80	30, 47, 71, 89	0
2	E	251/259 (96%)	-0.11	1 (0%) 93 95	28, 48, 68, 79	0
All	All	556/590 (94%)	-0.11	6 (1%) 82 86	28, 48, 70, 89	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	147	THR	3.7
2	B	245	PHE	3.1
2	E	148	TRP	2.9
2	B	148	TRP	2.4
1	A	14(K)	ILE	2.2
2	B	96	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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(Å ²)	Q<0.9
3	NAG	E	500	14/15	0.80	0.18	1.11	49,53,57,58	0
4	NA	B	1701	1/1	0.63	0.12	-0.02	54,54,54,54	0
4	NA	E	1702	1/1	0.63	0.12	-0.34	55,55,55,55	0
3	NAG	B	400	14/15	0.81	0.30	-	57,60,62,64	0

6.5 Other polymers

There are no such residues in this entry.