



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:24 PM BST

PDB ID : 5VI4  
Title : IL-33/ST2/IL-1RAcP ternary complex structure  
Authors : Guenther, S.; Sundberg, E.J.  
Deposited on : 2017-04-13  
Resolution : 2.79 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 : 2.13.1  
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) : 2.13.1

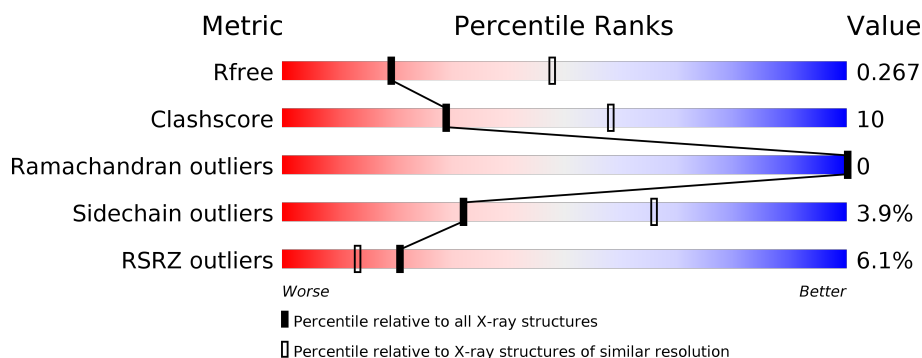
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	158	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	158	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	309	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>16%</div> <div>•</div> <div>22%</div> </div> </div>
2	E	309	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
3	C	339	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
3	F	339	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11304 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 Interleukin-33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1148	720	185	240	3			
1	D	146	Total	C	N	O	S	0	0	0
			1148	721	186	238	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	SER	CYS	engineered mutation	UNP Q8BVZ5
A	165	SER	CYS	engineered mutation	UNP Q8BVZ5
A	231	SER	CYS	engineered mutation	UNP Q8BVZ5
A	256	SER	CYS	engineered mutation	UNP Q8BVZ5
D	139	SER	CYS	engineered mutation	UNP Q8BVZ5
D	165	SER	CYS	engineered mutation	UNP Q8BVZ5
D	231	SER	CYS	engineered mutation	UNP Q8BVZ5
D	256	SER	CYS	engineered mutation	UNP Q8BVZ5

- Molecule 2 is a protein called Interleukin-1 receptor-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1901	1210	319	357	15			
2	E	260	Total	C	N	O	S	0	0	0
			2071	1317	352	387	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	GLU	-	expression tag	UNP P14719
B	25	THR	-	expression tag	UNP P14719
B	327	HIS	-	expression tag	UNP P14719
B	328	HIS	-	expression tag	UNP P14719

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Chain	Residue	Modelled	Actual	Comment	Reference
B	329	HIS	-	expression tag	UNP P14719
B	330	HIS	-	expression tag	UNP P14719
B	331	HIS	-	expression tag	UNP P14719
B	332	HIS	-	expression tag	UNP P14719
E	24	GLU	-	expression tag	UNP P14719
E	25	THR	-	expression tag	UNP P14719
E	327	HIS	-	expression tag	UNP P14719
E	328	HIS	-	expression tag	UNP P14719
E	329	HIS	-	expression tag	UNP P14719
E	330	HIS	-	expression tag	UNP P14719
E	331	HIS	-	expression tag	UNP P14719
E	332	HIS	-	expression tag	UNP P14719

- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2496	1594	423	463	16			
3	F	306	Total	C	N	O	S	0	0	0
			2498	1595	422	465	16			

There are 26 discrepancies between the modelled and reference sequences:

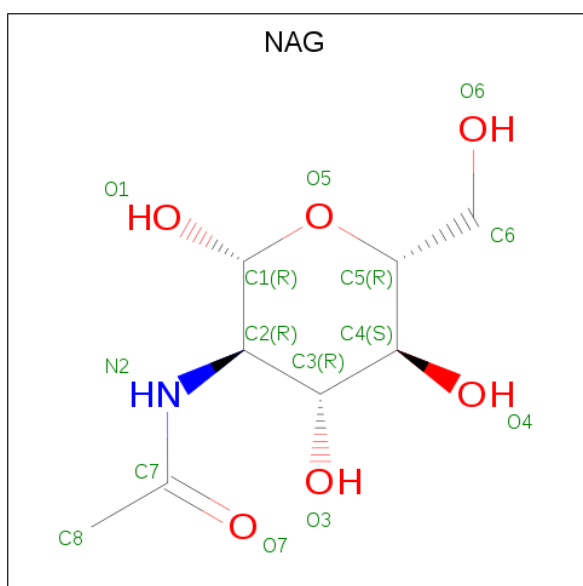
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLU	-	expression tag	UNP Q61730
C	19	THR	-	expression tag	UNP Q61730
C	20	GLY	-	expression tag	UNP Q61730
C	107	GLN	ASN	engineered mutation	UNP Q61730
C	111	GLN	ASN	engineered mutation	UNP Q61730
C	196	GLN	ASN	engineered mutation	UNP Q61730
C	209	GLN	ASN	engineered mutation	UNP Q61730
C	351	HIS	-	expression tag	UNP Q61730
C	352	HIS	-	expression tag	UNP Q61730
C	353	HIS	-	expression tag	UNP Q61730
C	354	HIS	-	expression tag	UNP Q61730
C	355	HIS	-	expression tag	UNP Q61730
C	356	HIS	-	expression tag	UNP Q61730
F	18	GLU	-	expression tag	UNP Q61730
F	19	THR	-	expression tag	UNP Q61730
F	20	GLY	-	expression tag	UNP Q61730
F	107	GLN	ASN	engineered mutation	UNP Q61730
F	111	GLN	ASN	engineered mutation	UNP Q61730

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	GLN	ASN	engineered mutation	UNP Q61730
F	209	GLN	ASN	engineered mutation	UNP Q61730
F	351	HIS	-	expression tag	UNP Q61730
F	352	HIS	-	expression tag	UNP Q61730
F	353	HIS	-	expression tag	UNP Q61730
F	354	HIS	-	expression tag	UNP Q61730
F	355	HIS	-	expression tag	UNP Q61730
F	356	HIS	-	expression tag	UNP Q61730

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

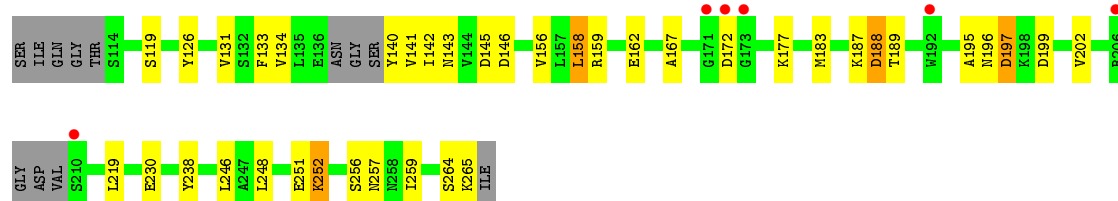


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

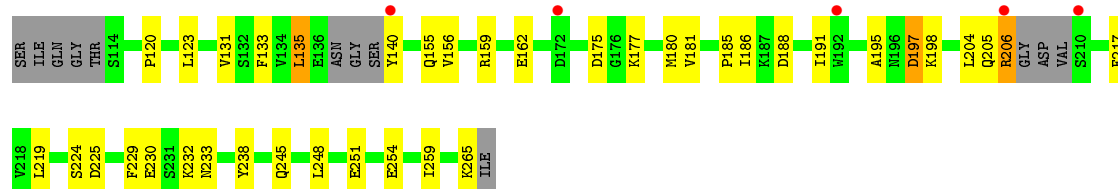
### 3 Residue-property plots [i](#)

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.

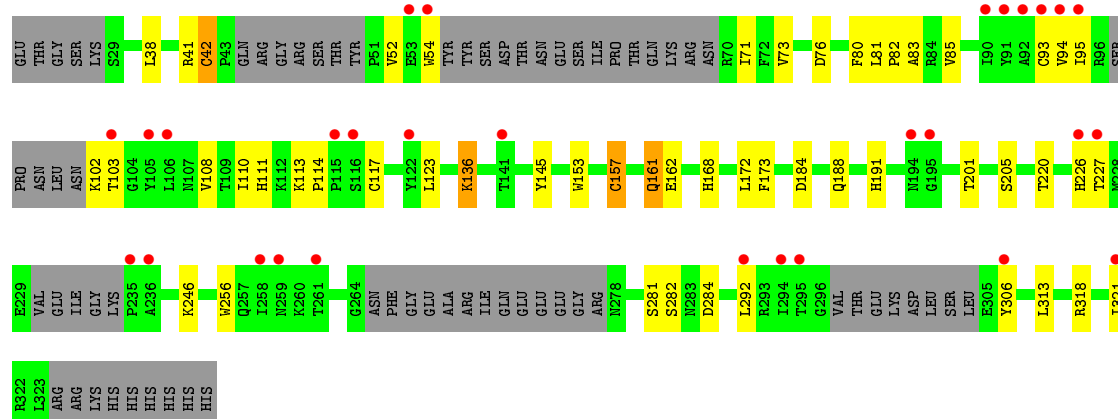
#### • Molecule 1: Interleukin-33



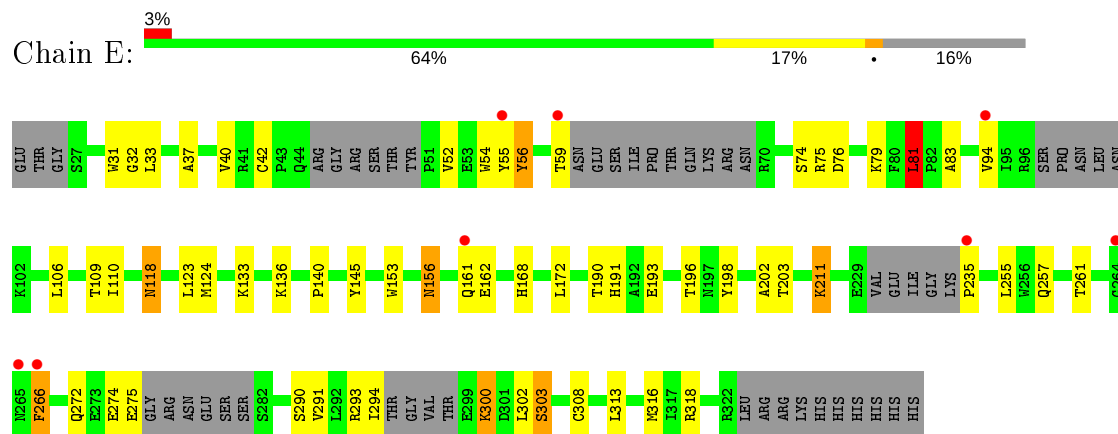
#### • Molecule 1: Interleukin-33



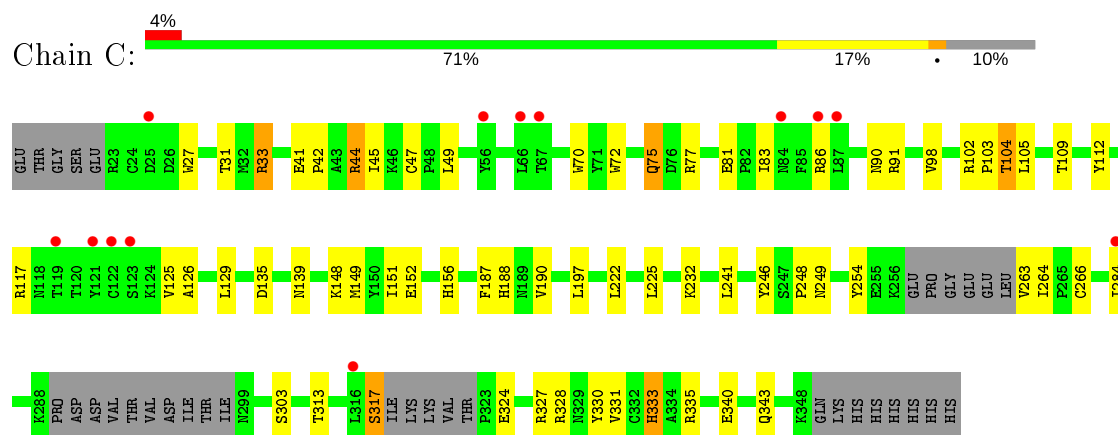
#### • Molecule 2: Interleukin-1 receptor-like 1



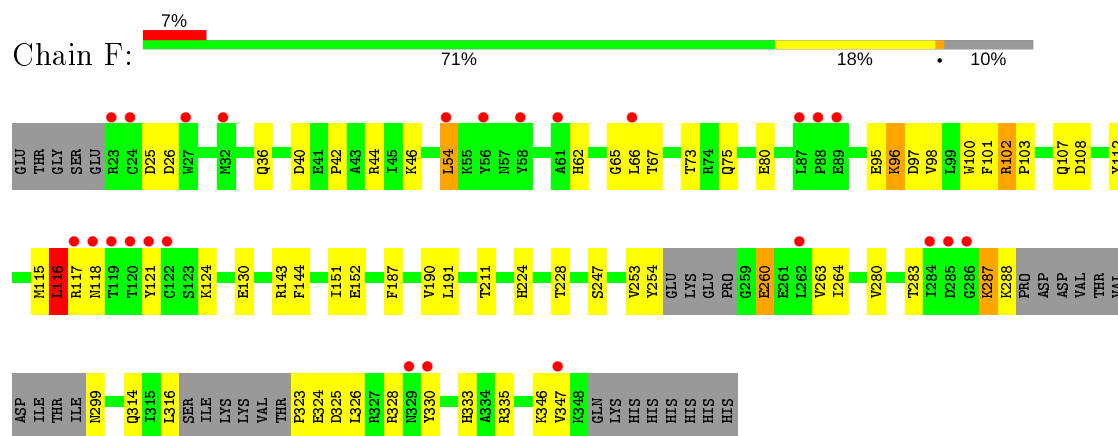
- Molecule 2: Interleukin-1 receptor-like 1



- Molecule 3: Interleukin-1 receptor accessory protein



- Molecule 3: Interleukin-1 receptor accessory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.31Å 107.33Å 176.04Å 90.00° 107.27° 90.00°	Depositor
Resolution (Å)	29.68 – 2.79 29.68 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.68-2.79) 99.0 (29.68-2.79)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.267 0.212 , 0.267	Depositor DCC
$R_{free}$ test set	2338 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.6	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	11304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/1168	0.69	2/1578 (0.1%)
1	D	0.44	0/1168	0.65	0/1577
2	B	0.38	0/1947	0.66	0/2644
2	E	0.45	0/2120	0.70	2/2873 (0.1%)
3	C	0.42	0/2564	0.69	2/3481 (0.1%)
3	F	0.44	0/2566	0.69	2/3486 (0.1%)
All	All	0.42	0/11533	0.68	8/15639 (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
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	94	VAL	CG1-CB-CG2	-8.52	97.27	110.90
2	E	81	LEU	CA-CB-CG	7.49	132.53	115.30
3	C	33	ARG	CA-CB-CG	7.43	129.76	113.40
1	A	252	LYS	CD-CE-NZ	-6.10	97.67	111.70
3	F	54	LEU	CA-CB-CG	5.78	128.59	115.30
3	F	116	LEU	CA-CB-CG	5.72	128.46	115.30
3	C	33	ARG	CB-CG-CD	-5.58	97.10	111.60
1	A	188	ASP	CB-CG-OD2	5.25	123.03	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ALA	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	1148	0	1099	26	0
1	D	1148	0	1106	28	0
2	B	1901	0	1797	43	0
2	E	2071	0	1969	41	0
3	C	2496	0	2409	47	0
3	F	2498	0	2400	44	0
4	B	14	0	13	0	0
4	E	28	0	26	0	0
All	All	11304	0	10819	212	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 (212) 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)
3:C:324:GLU:HA	3:C:327:ARG:NH1	1.75	1.01
2:E:235:PRO:HA	2:E:294:ILE:HD11	1.46	0.97
3:C:327:ARG:HH11	3:C:327:ARG:HG3	1.38	0.88
3:F:95:GLU:OE1	3:F:100:TRP:NE1	2.08	0.85
2:B:226:HIS:CD2	2:B:227:THR:H	1.96	0.84
3:C:151:ILE:HG12	3:C:152:GLU:HG3	1.59	0.82
3:C:284:ILE:HD11	3:C:330:TYR:CE2	2.16	0.80
3:F:151:ILE:HG12	3:F:152:GLU:HG3	1.64	0.79
3:C:27:TRP:HB2	3:C:125:VAL:HG22	1.64	0.78
2:E:52:VAL:HG21	2:E:76:ASP:HA	1.66	0.78
2:B:161:GLN:OE1	2:B:161:GLN:O	2.02	0.77
1:A:197:ASP:N	1:A:197:ASP:OD1	2.16	0.77
1:A:145:ASP:OD1	1:A:146:ASP:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:SER:HB2	2:E:211:LYS:HE3	1.66	0.76
2:E:83:ALA:HB1	2:E:110:ILE:HG12	1.67	0.76
2:E:235:PRO:CA	2:E:294:ILE:HD11	2.16	0.75
2:B:83:ALA:HB1	2:B:110:ILE:HD12	1.70	0.73
3:C:324:GLU:HA	3:C:327:ARG:HH11	1.53	0.72
2:B:161:GLN:O	2:B:162:GLU:HG3	1.91	0.70
3:F:66:LEU:HD12	3:F:118:ASN:HB3	1.75	0.69
3:F:95:GLU:HG2	3:F:96:LYS:HE3	1.76	0.68
2:E:140:PRO:HG2	2:E:202:ALA:HB1	1.75	0.68
2:E:133:LYS:HB2	2:E:211:LYS:HE2	1.76	0.67
1:A:195:ALA:HB1	1:A:248:LEU:HD11	1.75	0.67
1:A:172:ASP:HB2	3:C:303:SER:HB2	1.74	0.67
1:D:135:LEU:HD13	1:D:135:LEU:H	1.60	0.66
3:C:284:ILE:HD11	3:C:330:TYR:CD2	2.30	0.66
1:D:185:PRO:HD2	1:D:191:ILE:HG23	1.77	0.66
2:B:188:GLN:HB2	2:B:201:THR:HG22	1.78	0.66
1:A:134:VAL:HG22	1:A:141:VAL:HG22	1.80	0.63
2:B:220:THR:HG22	3:C:246:TYR:HB3	1.80	0.63
1:D:180:MET:HE2	1:D:232:LYS:HD2	1.80	0.63
2:B:145:TYR:HB3	2:B:191:HIS:HB2	1.81	0.62
3:F:330:TYR:CD1	3:F:347:VAL:HG21	2.34	0.62
3:F:67:THR:O	3:F:116:LEU:HA	2.00	0.62
1:A:251:GLU:C	1:A:252:LYS:HG2	2.20	0.62
3:F:187:PHE:HB2	3:F:190:VAL:HB	1.82	0.61
3:F:263:VAL:HA	3:F:316:LEU:O	2.00	0.61
3:C:187:PHE:HB2	3:C:190:VAL:HB	1.82	0.61
3:F:325:ASP:HA	3:F:328:ARG:HH11	1.64	0.61
2:B:226:HIS:HB3	2:B:321:ILE:CD1	2.30	0.61
2:B:42:CYS:CB	2:B:93:CYS:HG	2.13	0.61
3:C:263:VAL:HA	3:C:317:SER:HB2	1.83	0.61
2:B:226:HIS:CG	2:B:227:THR:H	2.18	0.60
3:C:31:THR:HG22	3:C:33:ARG:H	1.66	0.60
2:E:145:TYR:HB3	2:E:191:HIS:HB2	1.83	0.60
2:B:95:ILE:HG22	2:B:102:LYS:O	2.01	0.60
1:A:162:GLU:OE2	2:B:318:ARG:NH2	2.28	0.60
3:F:260:GLU:OE1	3:F:323:PRO:HD3	2.02	0.60
3:C:47:CYS:SG	3:C:49:LEU:HB2	2.43	0.59
3:F:253:VAL:HG22	3:F:346:LYS:HD3	1.84	0.59
3:F:73:THR:OG1	3:F:80:GLU:HG3	2.02	0.59
2:E:291:VAL:HG11	2:E:293:ARG:HH11	1.67	0.58
2:B:71:ILE:H	2:B:71:ILE:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD21	2:E:313:LEU:HD22	1.86	0.57
1:A:142:ILE:HD12	1:A:246:LEU:H	1.69	0.57
2:B:306:TYR:HB2	2:B:321:ILE:HG22	1.87	0.56
1:D:225:ASP:OD2	2:E:211:LYS:NZ	2.37	0.56
2:B:94:VAL:HG12	2:B:103:THR:HG22	1.86	0.56
2:B:168:HIS:HE1	3:C:187:PHE:O	1.88	0.56
2:B:113:LYS:HG3	2:B:114:PRO:HD2	1.88	0.56
1:D:162:GLU:OE2	2:E:318:ARG:NH1	2.38	0.56
2:B:226:HIS:CG	2:B:227:THR:N	2.71	0.56
2:E:161:GLN:O	2:E:162:GLU:HG3	2.05	0.56
2:E:81:LEU:HB3	2:E:198:TYR:CE1	2.42	0.55
3:C:151:ILE:CG1	3:C:152:GLU:HG3	2.35	0.55
2:B:38:LEU:HD23	2:B:80:PHE:CD2	2.42	0.55
3:C:135:ASP:HB3	3:C:139:ASN:H	1.72	0.54
2:E:33:LEU:HD21	2:E:123:LEU:HD13	1.88	0.54
2:B:85:VAL:HA	2:B:110:ILE:HB	1.89	0.54
3:F:115:MET:HE2	3:F:117:ARG:HD2	1.89	0.54
1:A:134:VAL:CG2	1:A:141:VAL:HG22	2.37	0.54
3:C:327:ARG:HG3	3:C:327:ARG:NH1	2.09	0.54
1:D:180:MET:HE2	1:D:232:LYS:CD	2.38	0.54
3:F:324:GLU:OE1	3:F:324:GLU:N	2.36	0.53
3:F:65:GLY:O	3:F:66:LEU:HD12	2.08	0.53
1:D:120:PRO:HB3	1:D:186:ILE:HD11	1.91	0.53
2:E:302:LEU:HD12	2:E:302:LEU:H	1.72	0.53
3:F:325:ASP:OD1	3:F:328:ARG:NH1	2.42	0.53
3:C:331:VAL:HG12	3:C:333:HIS:CE1	2.44	0.52
2:B:52:VAL:HG11	2:B:76:ASP:HA	1.90	0.52
2:B:246:LYS:HD3	3:C:241:LEU:HD21	1.92	0.51
1:D:155:GLN:HB3	1:D:186:ILE:HG13	1.92	0.51
3:C:41:GLU:O	3:C:104:THR:HB	2.10	0.51
2:B:256:TRP:CD1	2:B:292:LEU:HB2	2.45	0.51
1:D:188:ASP:O	1:D:191:ILE:HG22	2.11	0.51
2:E:300:LYS:O	2:E:303:SER:HB3	2.11	0.51
3:F:108:ASP:HB3	3:F:112:TYR:OH	2.11	0.51
2:E:272:GLN:OE1	2:E:290:SER:OG	2.19	0.50
3:C:266:CYS:O	3:C:313:THR:HA	2.12	0.50
3:C:148:LYS:HA	3:C:232:LYS:O	2.11	0.50
2:E:168:HIS:CE1	3:F:191:LEU:HB2	2.46	0.50
3:C:77:ARG:NH1	3:C:81:GLU:OE1	2.45	0.49
2:E:308:CYS:O	2:E:318:ARG:HA	2.12	0.49
3:F:323:PRO:HG2	3:F:324:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:TYR:O	2:E:59:THR:HG23	2.13	0.49
2:E:257:GLN:OE1	2:E:318:ARG:NH2	2.45	0.49
2:E:156:ASN:O	2:E:156:ASN:ND2	2.43	0.49
1:A:143:ASN:OD1	2:B:41:ARG:NH2	2.45	0.49
3:F:326:LEU:H	3:F:326:LEU:HD12	1.77	0.49
2:E:31:TRP:HA	2:E:109:THR:O	2.12	0.49
2:E:42:CYS:HB2	2:E:54:TRP:CZ2	2.48	0.49
1:A:219:LEU:HD21	2:B:313:LEU:HD22	1.95	0.48
2:B:306:TYR:HB2	2:B:321:ILE:CG2	2.43	0.48
3:F:25:ASP:N	3:F:25:ASP:OD2	2.34	0.48
3:C:45:ILE:HD13	3:C:129:LEU:HD12	1.94	0.48
1:A:251:GLU:HG3	1:A:259:ILE:HD11	1.95	0.48
1:D:175:ASP:OD2	1:D:177:LYS:NZ	2.45	0.48
1:A:256:SER:HB2	3:C:188:HIS:NE2	2.29	0.48
2:B:153:TRP:CE2	2:B:172:LEU:HB2	2.48	0.48
2:B:184:ASP:OD1	2:B:205:SER:HB3	2.13	0.48
3:F:115:MET:HB2	3:F:124:LYS:HB2	1.96	0.48
2:B:281:SER:OG	2:B:282:SER:N	2.47	0.47
2:E:74:SER:HB2	2:E:79:LYS:HE3	1.96	0.47
3:F:46:LYS:HD2	3:F:97:ASP:OD2	2.15	0.47
3:C:328:ARG:HB2	3:C:330:TYR:CE1	2.49	0.47
3:C:75:GLN:HB2	3:C:109:THR:HG22	1.97	0.47
3:C:335:ARG:HB2	3:C:340:GLU:HG3	1.95	0.47
2:E:294:ILE:HD12	2:E:294:ILE:O	2.15	0.47
3:F:62:HIS:O	3:F:62:HIS:ND1	2.47	0.47
3:F:26:ASP:HB3	3:F:124:LYS:HE3	1.96	0.47
3:C:324:GLU:HA	3:C:327:ARG:HH12	1.74	0.47
3:F:280:VAL:HG13	3:F:314:GLN:NE2	2.30	0.46
1:A:202:VAL:HB	1:A:246:LEU:HB3	1.97	0.46
3:C:44:ARG:HB2	3:C:98:VAL:HG11	1.96	0.46
3:C:90:ASN:ND2	3:C:90:ASN:O	2.49	0.46
1:D:195:ALA:HB1	1:D:248:LEU:HD11	1.96	0.46
1:D:251:GLU:HG3	1:D:259:ILE:HD11	1.97	0.46
3:F:42:PRO:HA	3:F:101:PHE:O	2.15	0.46
3:F:95:GLU:O	3:F:96:LYS:HG2	2.15	0.46
3:F:67:THR:HG22	3:F:117:ARG:O	2.16	0.46
2:B:281:SER:HB2	3:C:249:ASN:HB2	1.97	0.46
3:C:125:VAL:HG12	3:C:126:ALA:N	2.30	0.45
2:E:124:MET:HE2	2:E:203:THR:HG22	1.98	0.45
2:B:42:CYS:CB	2:B:93:CYS:SG	3.03	0.45
3:F:44:ARG:HB2	3:F:98:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:CG	1:A:199:ASP:HB3	2.37	0.45
2:B:71:ILE:HG13	2:B:80:PHE:CD1	2.52	0.45
2:B:42:CYS:HB2	2:B:93:CYS:SG	2.57	0.45
2:E:37:ALA:HB2	2:E:198:TYR:CB	2.46	0.45
3:C:248:PRO:O	3:C:343:GLN:HG2	2.17	0.45
2:E:118:ASN:N	2:E:118:ASN:OD1	2.49	0.45
2:E:153:TRP:CE2	2:E:172:LEU:HB2	2.51	0.45
3:F:254:TYR:CZ	3:F:264:ILE:HG23	2.51	0.45
3:C:149:MET:HG3	3:C:156:HIS:CD2	2.51	0.45
1:D:180:MET:CE	1:D:232:LYS:HD2	2.47	0.45
3:C:284:ILE:HA	3:C:284:ILE:HD13	1.88	0.45
3:C:112:TYR:O	3:C:126:ALA:HA	2.17	0.44
1:D:191:ILE:HD12	1:D:205:GLN:C	2.36	0.44
3:C:125:VAL:HG12	3:C:126:ALA:H	1.83	0.44
3:F:287:LYS:HE2	3:F:288:LYS:NZ	2.32	0.44
3:C:254:TYR:CZ	3:C:264:ILE:HG23	2.53	0.44
1:A:131:VAL:HA	1:A:143:ASN:O	2.18	0.43
2:E:193:GLU:O	2:E:196:THR:OG1	2.27	0.43
3:F:211:THR:HG23	3:F:228:THR:HG23	1.98	0.43
3:F:66:LEU:HD12	3:F:66:LEU:HA	1.81	0.43
2:E:274:GLU:HG2	2:E:275:GLU:H	1.83	0.43
2:E:32:GLY:O	2:E:110:ILE:HA	2.19	0.43
1:A:142:ILE:HD13	1:A:246:LEU:HB2	2.00	0.43
3:F:42:PRO:HD2	3:F:224:HIS:O	2.19	0.43
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.83	0.43
1:D:123:LEU:HB3	1:D:131:VAL:CG1	2.49	0.43
1:A:140:TYR:HE1	1:A:188:ASP:OD1	2.02	0.43
3:C:42:PRO:HG2	3:C:225:LEU:HD21	2.00	0.43
3:F:95:GLU:OE1	3:F:100:TRP:CD1	2.70	0.43
1:D:230:GLU:HB2	1:D:238:TYR:CE2	2.54	0.42
1:D:135:LEU:HA	1:D:140:TYR:HA	2.00	0.42
2:E:42:CYS:HB2	2:E:54:TRP:CH2	2.54	0.42
2:B:111:HIS:CD2	2:B:123:LEU:HD21	2.54	0.42
3:C:222:LEU:HD12	3:C:222:LEU:HA	1.70	0.42
2:E:37:ALA:HB2	2:E:198:TYR:HB2	2.01	0.42
1:A:143:ASN:HD21	2:B:41:ARG:NH2	2.18	0.42
1:A:158:LEU:HD12	1:A:183:MET:HG2	2.00	0.42
1:D:188:ASP:OD2	1:D:206:ARG:NH2	2.52	0.42
3:F:283:THR:HG23	3:F:333:HIS:CD2	2.54	0.42
1:D:133:PHE:CE2	1:D:156:VAL:HG12	2.54	0.42
1:D:217:PHE:HB3	1:D:229:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CE1	1:A:156:VAL:HG12	2.55	0.42
2:B:117:CYS:HB3	2:B:157:CYS:HB2	1.92	0.42
2:B:81:LEU:HA	2:B:82:PRO:HA	1.77	0.42
1:D:197:ASP:OD1	1:D:233:ASN:ND2	2.48	0.42
1:A:159:ARG:NH2	1:A:189:THR:HG22	2.35	0.42
1:D:254:GLU:HA	3:F:187:PHE:CD1	2.54	0.42
2:B:80:PHE:HE2	2:B:108:VAL:HG11	1.84	0.42
2:B:94:VAL:HG12	2:B:103:THR:CG2	2.50	0.42
1:D:159:ARG:O	1:D:181:VAL:HA	2.21	0.41
2:E:40:VAL:CG1	2:E:106:LEU:HD22	2.51	0.41
2:E:136:LYS:HE2	2:E:136:LYS:HB3	1.80	0.41
3:C:335:ARG:NH2	3:C:340:GLU:OE2	2.53	0.41
3:C:49:LEU:HA	3:C:49:LEU:HD23	1.85	0.41
3:F:66:LEU:CD1	3:F:118:ASN:HB3	2.47	0.41
3:F:115:MET:CE	3:F:117:ARG:HD2	2.49	0.41
2:B:136:LYS:HG3	2:B:173:PHE:CE1	2.56	0.41
1:D:191:ILE:HG13	1:D:204:LEU:HD22	2.01	0.41
1:D:162:GLU:CD	2:E:316:MET:HE1	2.40	0.41
1:A:126:TYR:CD1	1:A:257:ASN:HB2	2.56	0.41
2:B:226:HIS:HB3	2:B:321:ILE:HD11	2.02	0.41
2:B:54:TRP:CG	2:B:73:VAL:HG21	2.56	0.41
1:A:230:GLU:HB2	1:A:238:TYR:CE2	2.55	0.41
3:C:102:ARG:HA	3:C:103:PRO:HA	1.81	0.41
3:F:102:ARG:HA	3:F:103:PRO:HA	1.65	0.41
1:A:251:GLU:O	1:A:252:LYS:HG2	2.20	0.41
2:B:161:GLN:CD	2:B:161:GLN:O	2.59	0.41
3:C:70:TRP:HB3	3:C:83:ILE:HD12	2.03	0.40
1:D:265:LYS:HA	1:D:265:LYS:HD3	1.80	0.40
2:E:124:MET:CE	2:E:203:THR:HG22	2.52	0.40
3:C:91:ARG:CZ	3:C:105:LEU:HD12	2.52	0.40
3:F:36:GLN:HE22	3:F:143:ARG:HG3	1.86	0.40
3:F:36:GLN:HA	3:F:130:GLU:O	2.22	0.40
1:A:156:VAL:HG23	1:A:158:LEU:HD13	2.03	0.40
2:E:261:THR:HG21	2:E:266:PHE:HB2	2.04	0.40
3:F:66:LEU:HD21	3:F:121:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/158 (89%)	137 (98%)	3 (2%)	0	100	100
1	D	140/158 (89%)	137 (98%)	3 (2%)	0	100	100
2	B	228/309 (74%)	217 (95%)	11 (5%)	0	100	100
2	E	246/309 (80%)	229 (93%)	17 (7%)	0	100	100
3	C	297/339 (88%)	287 (97%)	10 (3%)	0	100	100
3	F	298/339 (88%)	289 (97%)	9 (3%)	0	100	100
All	All	1349/1612 (84%)	1296 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	134/144 (93%)	127 (95%)	7 (5%)	23	55
1	D	134/144 (93%)	129 (96%)	5 (4%)	34	68
2	B	210/278 (76%)	205 (98%)	5 (2%)	49	81
2	E	228/278 (82%)	216 (95%)	12 (5%)	22	54
3	C	283/316 (90%)	275 (97%)	8 (3%)	43	77
3	F	282/316 (89%)	269 (95%)	13 (5%)	27	60
All	All	1271/1476 (86%)	1221 (96%)	50 (4%)	32	66



All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	158	LEU
1	A	177	LYS
1	A	187	LYS
1	A	197	ASP
1	A	264	SER
1	A	265	LYS
2	B	42	CYS
2	B	136	LYS
2	B	157	CYS
2	B	161	GLN
2	B	284	ASP
3	C	44	ARG
3	C	72	TRP
3	C	75	GLN
3	C	86	ARG
3	C	104	THR
3	C	117	ARG
3	C	317	SER
3	C	333	HIS
1	D	135	LEU
1	D	197	ASP
1	D	198	LYS
1	D	206	ARG
1	D	245	GLN
2	E	55	TYR
2	E	56	TYR
2	E	75	ARG
2	E	81	LEU
2	E	118	ASN
2	E	156	ASN
2	E	190	THR
2	E	211	LYS
2	E	255	LEU
2	E	266	PHE
2	E	300	LYS
2	E	303	SER
3	F	40	ASP
3	F	54	LEU
3	F	75	GLN
3	F	96	LYS
3	F	102	ARG

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Mol	Chain	Res	Type
3	F	107	GLN
3	F	116	LEU
3	F	144	PHE
3	F	247	SER
3	F	260	GLU
3	F	287	LYS
3	F	299	ASN
3	F	335	ARG

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	161	GLN
2	B	168	HIS
2	B	226	HIS
2	B	283	ASN
3	C	133	GLN
3	C	206	ASN
3	C	329	ASN
1	D	194	HIS
1	D	205	GLN
3	F	36	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](#)

3 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	$\# Z  > 2$
4	NAG	E	402	2	14,14,15	1.02	1 (7%)	17,19,21	2.60	7 (41%)
4	NAG	E	401	2	14,14,15	0.34	0	17,19,21	1.27	2 (11%)
4	NAG	B	401	2	14,14,15	0.35	0	17,19,21	1.14	1 (5%)

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	402	2	-	4/6/23/26	0/1/1/1
4	NAG	E	401	2	-	3/6/23/26	0/1/1/1
4	NAG	B	401	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	402	NAG	C2-N2	-2.02	1.42	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	402	NAG	C1-O5-C5	-7.49	102.04	112.19
4	E	402	NAG	O5-C5-C6	3.30	112.37	107.20
4	B	401	NAG	C1-C2-N2	-2.98	105.40	110.49
4	E	402	NAG	O4-C4-C5	2.73	116.08	109.30
4	E	402	NAG	O5-C1-C2	2.73	115.60	111.29
4	E	402	NAG	C6-C5-C4	-2.63	106.85	113.00
4	E	402	NAG	O3-C3-C4	-2.47	104.65	110.35
4	E	401	NAG	C6-C5-C4	-2.24	107.76	113.00
4	E	401	NAG	C1-O5-C5	-2.19	109.23	112.19
4	E	402	NAG	C1-C2-N2	-2.13	106.84	110.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	402	NAG	C8-C7-N2-C2
4	E	402	NAG	O7-C7-N2-C2
4	E	401	NAG	C3-C2-N2-C7
4	E	401	NAG	C8-C7-N2-C2
4	E	401	NAG	O7-C7-N2-C2
4	E	402	NAG	C1-C2-N2-C7
4	B	401	NAG	C1-C2-N2-C7
4	B	401	NAG	C3-C2-N2-C7
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2
4	E	402	NAG	C4-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(Å²)	Q<0.9
1	A	146/158 (92%)	0.22	6 (4%)	37	27	48, 71, 118, 126	0
1	D	146/158 (92%)	0.11	5 (3%)	45	35	40, 66, 133, 157	0
2	B	242/309 (78%)	0.59	29 (11%)	4	2	43, 81, 128, 174	0
2	E	260/309 (84%)	0.19	8 (3%)	49	39	41, 70, 123, 148	0
3	C	305/339 (89%)	0.04	13 (4%)	35	25	32, 63, 122, 153	0
3	F	306/339 (90%)	0.26	25 (8%)	11	6	35, 67, 140, 167	0
All	All	1405/1612 (87%)	0.24	86 (6%)	21	13	32, 69, 128, 174	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	121	TYR	7.9
3	F	119	THR	6.0
2	B	90	ILE	5.2
3	C	122	CYS	4.8
2	B	94	VAL	4.4
2	B	54	TRP	4.2
2	B	53	GLU	4.2
2	B	92	ALA	4.2
3	C	119	THR	4.2
2	B	115	PRO	4.1
2	B	103	THR	4.1
3	F	88	PRO	4.0
1	D	210	SER	4.0
3	F	58	TYR	3.9
2	B	105	TYR	3.7
2	B	93	CYS	3.7
2	B	306	TYR	3.7
2	E	265	ASN	3.7
3	C	56	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	89	GLU	3.7
2	B	226	HIS	3.7
1	A	210	SER	3.6
3	C	121	TYR	3.4
3	F	56	TYR	3.4
1	D	140	TYR	3.4
2	B	295	THR	3.3
2	E	266	PHE	3.3
2	B	122	TYR	3.3
2	B	294	ILE	3.2
2	B	235	PRO	3.2
1	A	172	ASP	3.2
3	F	118	ASN	3.1
3	F	27	TRP	3.1
3	F	286	GLY	3.0
2	B	91	TYR	3.0
3	F	120	THR	2.9
2	B	95	ILE	2.9
2	B	116	SER	2.9
2	B	227	THR	2.8
1	D	172	ASP	2.8
2	E	235	PRO	2.8
2	E	59	THR	2.8
2	B	195	GLY	2.8
2	E	94	VAL	2.7
3	C	67	THR	2.7
3	C	87	LEU	2.6
3	C	284	ILE	2.6
1	A	192	TRP	2.6
1	A	206	ARG	2.6
3	F	262	LEU	2.6
3	C	86	ARG	2.6
2	E	161	GLN	2.5
3	F	87	LEU	2.4
2	B	292	LEU	2.4
3	F	122	CYS	2.4
3	F	347	VAL	2.4
3	F	284	ILE	2.4
3	F	66	LEU	2.3
3	C	84	ASN	2.3
1	A	171	GLY	2.3
3	F	32	MET	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	117	ARG	2.3
2	B	106	LEU	2.3
2	B	258	ILE	2.3
2	B	261	THR	2.2
3	F	330	TYR	2.2
3	F	23	ARG	2.2
2	B	321	ILE	2.2
3	F	24	CYS	2.2
3	C	123	SER	2.2
2	B	194	ASN	2.1
3	F	285	ASP	2.1
2	E	264	GLY	2.1
3	F	329	ASN	2.1
2	B	141	THR	2.1
2	B	259	ASN	2.1
3	F	54	LEU	2.1
3	F	61	ALA	2.1
1	D	206	ARG	2.1
3	C	316	LEU	2.1
3	C	25	ASP	2.0
2	B	236	ALA	2.0
1	A	173	GLY	2.0
2	E	55	TYR	2.0
1	D	192	TRP	2.0
3	C	66	LEU	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	401	14/15	0.88	0.20	80,100,105,107	0
4	NAG	E	402	14/15	0.91	0.24	58,71,79,86	0
4	NAG	B	401	14/15	0.93	0.23	60,77,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.