



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 06:21 AM EDT

PDB ID : 7N2Q
Title : AS4.3-YEIH-HLA*B27
Authors : Yang, X.; Jude, K.M.; Garcia, K.C.
Deposited on : 2021-05-29
Resolution : 2.70 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

<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>.

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)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

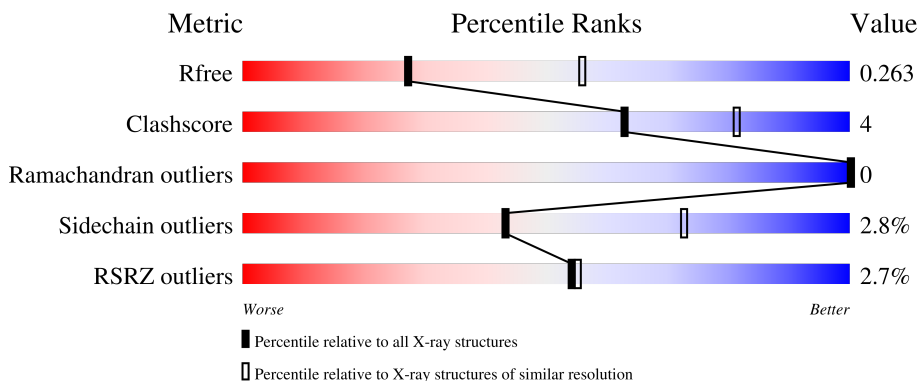
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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	D	204	 9% 88% 8% ..
1	E	204	 3% 87% 11% .
2	F	241	 2% 86% 12% ..
2	G	241	 2% 84% 15% .
3	A	278	 1% 84% 14% ..

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Mol	Chain	Length	Quality of chain
3	H	278	 <p>87% 12%</p>
4	B	100	 <p>83% 15%</p>
4	I	100	 <p>87% 12%</p>
5	C	9	 <p>100%</p>
5	J	9	 <p>89% 11%</p>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13409 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 AS4.3 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	201	1551	967	260	317	7	0	0	0
1	E	201	1551	967	260	317	7	0	0	0

- Molecule 2 is a protein called AS4.3 T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	238	1893	1198	326	364	5	0	0	0
2	G	240	1909	1207	331	366	5	0	0	0

- Molecule 3 is a protein called Human leukocyte antigen B27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	276	2251	1401	408	436	6	0	0	0
3	H	276	2251	1401	408	436	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	SER	CYS	conflict	UNP A3F718
H	67	SER	CYS	conflict	UNP A3F718

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	100	834	531	141	159	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	99	829	528	140	158	3	0	0	0

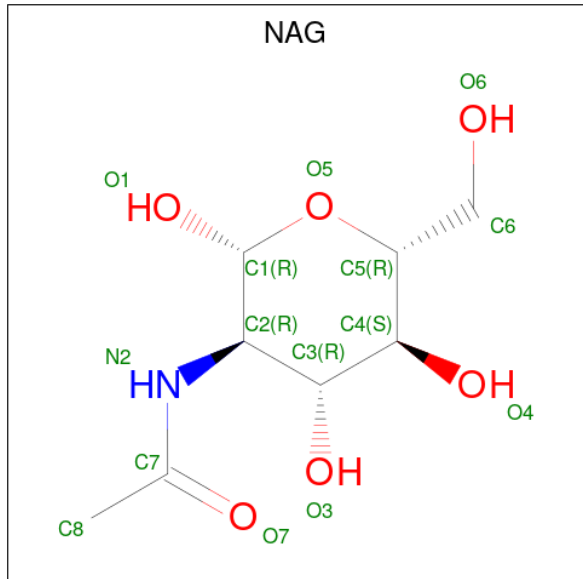
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
I	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called YeiH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	9	74	50	12	10	2	0	0	0
5	J	9	74	50	12	10	2	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



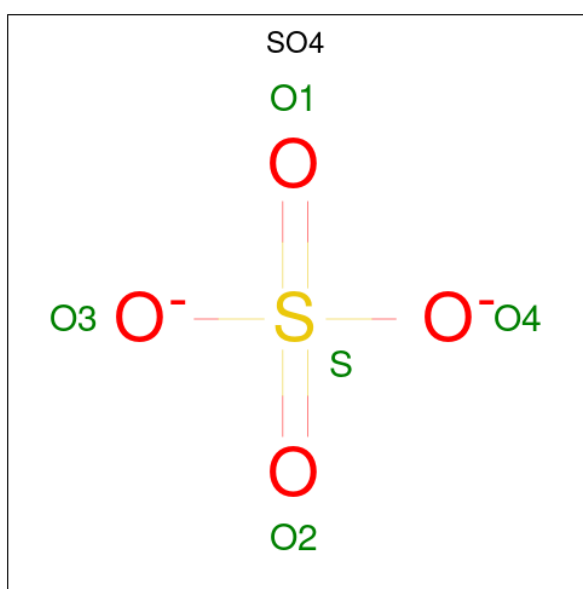
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
6	D	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	O S	0	0
			5	4 1		
7	E	1	Total	O S	0	0
			5	4 1		
7	G	1	Total	O S	0	0
			5	4 1		
7	H	1	Total	O S	0	0
			5	4 1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0

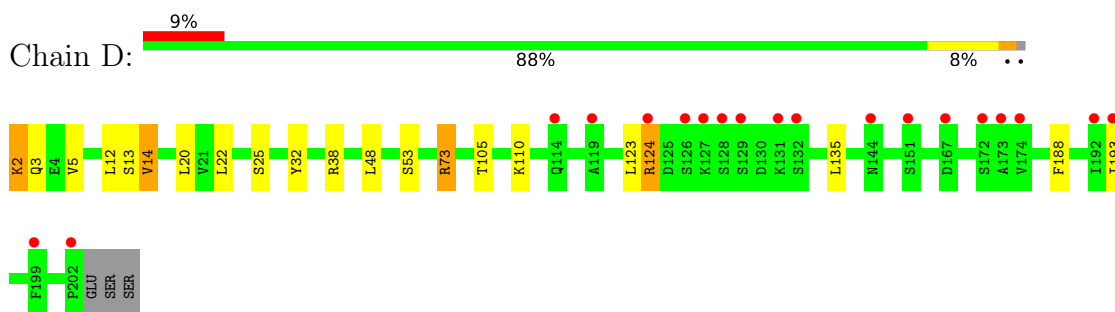
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	4	Total O 4 4	0	0
9	F	5	Total O 5 5	0	0
9	A	14	Total O 14 14	0	0
9	B	3	Total O 3 3	0	0
9	C	2	Total O 2 2	0	0
9	E	11	Total O 11 11	0	0
9	G	8	Total O 8 8	0	0
9	H	20	Total O 20 20	0	0
9	I	3	Total O 3 3	0	0

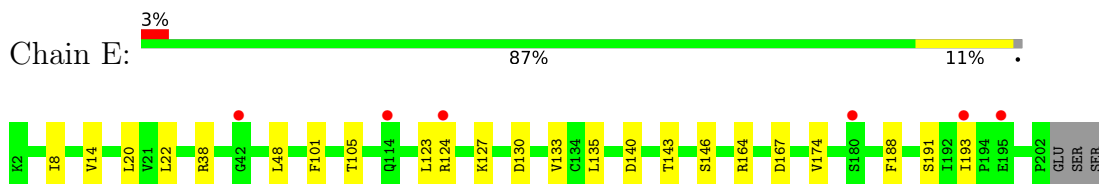
3 Residue-property plots [i](#)

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.

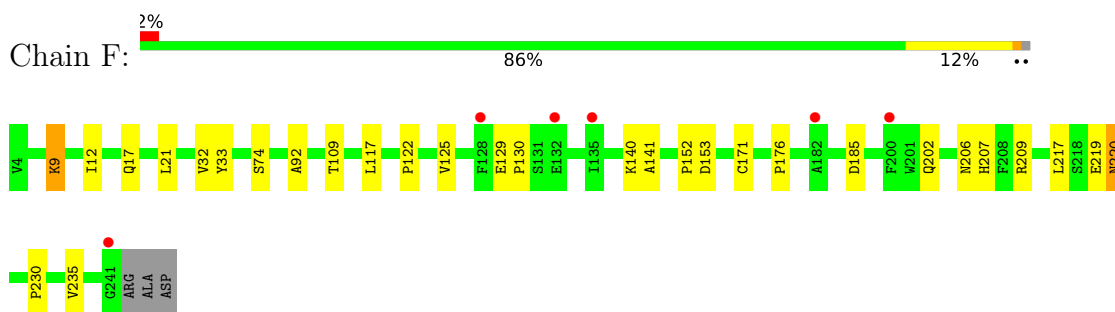
- Molecule 1: AS4.3 T cell receptor alpha chain



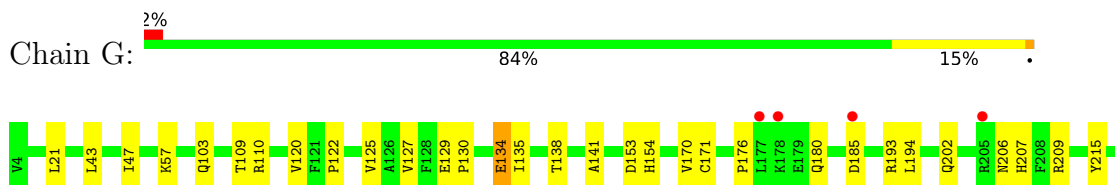
- Molecule 1: AS4.3 T cell receptor alpha chain

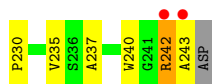


- Molecule 2: AS4.3 T cell receptor beta chain

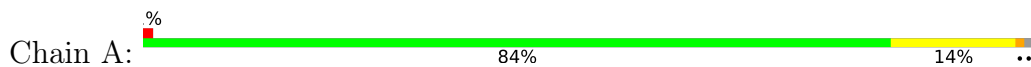


- Molecule 2: AS4.3 T cell receptor beta chain

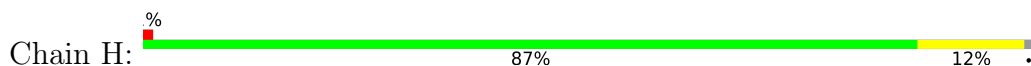




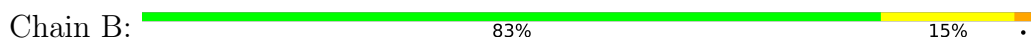
- Molecule 3: Human leukocyte antigen B27



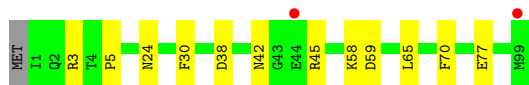
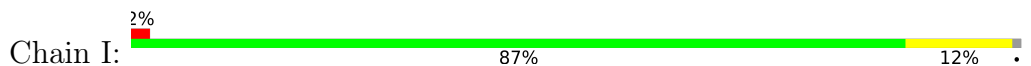
- Molecule 3: Human leukocyte antigen B27



- Molecule 4: Beta-2-microglobulin



- Molecule 4: Beta-2-microglobulin

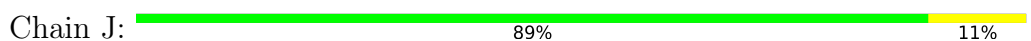


- Molecule 5: YeiH protein



There are no outlier residues recorded for this chain.

- Molecule 5: YeiH protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.98Å 97.41Å 175.48Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	47.42 – 2.70 47.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.42-2.70) 97.0 (47.42-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.213 , 0.264 0.214 , 0.263	Depositor DCC
R_{free} test set	2001 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13409	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.333 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, SO4, 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	D	0.25	0/1582	0.46	0/2146
1	E	0.26	0/1582	0.46	0/2146
2	F	0.25	0/1944	0.50	0/2652
2	G	0.25	0/1960	0.50	0/2673
3	A	0.24	0/2313	0.51	0/3147
3	H	0.24	0/2313	0.54	1/3147 (0.0%)
4	B	0.24	0/857	0.48	0/1159
4	I	0.23	0/852	0.46	0/1152
5	C	0.25	0/75	0.54	0/98
5	J	0.26	0/75	0.53	0/98
All	All	0.25	0/13553	0.50	1/18418 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	274	TRP	C-N-CA	7.21	139.72	121.70

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	D	1551	0	1485	12	0
1	E	1551	0	1485	17	0
2	F	1893	0	1797	17	0
2	G	1909	0	1815	21	0
3	A	2251	0	2109	21	0
3	H	2251	0	2109	15	0
4	B	834	0	796	11	0
4	I	829	0	794	6	0
5	C	74	0	85	0	0
5	J	74	0	85	1	0
6	D	28	0	26	0	0
6	E	28	0	26	1	0
6	F	14	0	13	0	0
6	G	14	0	13	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
7	G	5	0	0	0	0
7	H	5	0	0	0	0
8	E	6	0	8	0	0
8	G	12	0	16	1	0
9	A	14	0	0	0	0
9	B	3	0	0	0	0
9	C	2	0	0	0	0
9	D	4	0	0	0	0
9	E	11	0	0	0	0
9	F	5	0	0	0	0
9	G	8	0	0	0	0
9	H	20	0	0	1	0
9	I	3	0	0	0	0
All	All	13409	0	12662	111	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 4.

All (111) 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:F:9:LYS:H	2:F:9:LYS:HD3	1.38	0.87
1:E:14:VAL:HG21	1:E:20:LEU:HD21	1.75	0.69
3:A:266:LEU:HD13	3:A:270:LEU:HD13	1.76	0.67
4:B:19:LYS:HE3	4:B:20:SER:H	1.61	0.66
1:D:2:LYS:HZ2	1:D:3:GLN:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:71:THR:HG21	1:E:130:ASP:HB3	1.77	0.64
4:B:24:ASN:HB3	4:B:65:LEU:HD11	1.82	0.61
3:H:266:LEU:HD13	3:H:270:LEU:HD13	1.83	0.60
3:H:75:ARG:NH1	9:H:401:HOH:O	2.34	0.60
2:F:153:ASP:HB2	2:F:176:PRO:HG2	1.83	0.60
1:D:124:ARG:HG2	2:F:129:GLU:HB2	1.85	0.59
3:A:14:ARG:HB3	3:A:17:ARG:HB2	1.84	0.59
3:A:268:LYS:HD2	3:A:269:PRO:HD2	1.84	0.59
3:H:258:THR:HG22	3:H:273:ARG:HD3	1.85	0.58
2:F:125:VAL:HG22	2:F:235:VAL:HG12	1.86	0.58
4:I:58:LYS:HD2	4:I:58:LYS:H	1.68	0.58
2:G:153:ASP:HB2	2:G:176:PRO:HG2	1.84	0.58
3:A:177:GLU:HG2	3:A:178:THR:HG23	1.85	0.57
2:G:125:VAL:HG22	2:G:235:VAL:HG12	1.86	0.57
3:H:177:GLU:HG2	3:H:178:THR:HG23	1.86	0.57
2:G:122:PRO:HD3	2:G:230:PRO:HB3	1.86	0.57
2:F:122:PRO:HD3	2:F:230:PRO:HB3	1.86	0.57
3:A:262:GLN:HG2	3:A:269:PRO:HB3	1.87	0.57
1:E:146:SER:H	1:E:191:SER:HB2	1.70	0.56
1:E:124:ARG:HG2	2:G:129:GLU:HB2	1.88	0.56
1:D:13:SER:HB2	1:D:110:LYS:HE3	1.86	0.56
2:F:117:LEU:HD13	2:F:217:LEU:HD22	1.88	0.56
3:H:5:MET:HB2	3:H:168:LEU:HD13	1.88	0.56
4:I:24:ASN:HB3	4:I:65:LEU:HD11	1.89	0.55
1:E:22:LEU:HD22	1:E:105:THR:HG21	1.90	0.54
2:G:130:PRO:HG2	2:G:141:ALA:HB1	1.90	0.54
3:A:78:LEU:HG	3:A:95:LEU:HD12	1.89	0.53
2:G:21:LEU:HD22	2:G:109:THR:HG21	1.90	0.53
2:F:9:LYS:HD3	2:F:9:LYS:N	2.17	0.53
1:D:123:LEU:HD23	2:F:130:PRO:HA	1.90	0.53
1:E:164:ARG:NH2	1:E:167:ASP:OD1	2.42	0.53
1:D:188:PHE:HB2	1:D:193:ILE:HD11	1.90	0.52
3:A:84:TYR:OH	3:A:146:LYS:NZ	2.38	0.52
1:D:22:LEU:HD22	1:D:105:THR:HG21	1.91	0.52
1:E:188:PHE:HB2	1:E:193:ILE:HD11	1.91	0.52
2:F:130:PRO:HG2	2:F:141:ALA:HB1	1.92	0.52
3:A:106:ASP:OD1	3:A:106:ASP:N	2.36	0.51
2:G:134:GLU:HG3	2:G:135:ILE:N	2.25	0.51
1:E:38:ARG:HB3	1:E:48:LEU:HD11	1.94	0.50
2:G:103:GLN:HG3	8:G:302:GOL:H31	1.93	0.50
1:D:14:VAL:HG11	1:D:20:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:220:ASN:OD1	2:F:220:ASN:N	2.44	0.50
4:B:48:LYS:HE3	1:E:127:LYS:HE3	1.93	0.50
4:B:5:PRO:HB3	4:B:30:PHE:HB3	1.93	0.50
3:A:230:LEU:HD11	3:A:243:LYS:HE3	1.95	0.49
3:H:202:ARG:HG3	3:H:246:ALA:HB2	1.93	0.49
2:F:33:TYR:HB2	2:F:92:ALA:HB3	1.95	0.49
3:A:224:GLN:O	3:A:228:THR:OG1	2.12	0.49
2:G:127:VAL:HG13	2:G:237:ALA:HB3	1.94	0.49
3:A:226:GLN:H	3:A:226:GLN:CD	2.16	0.49
1:D:38:ARG:HB3	1:D:48:LEU:HD11	1.94	0.48
3:A:261:VAL:HG13	3:A:270:LEU:HB2	1.94	0.48
2:F:207:HIS:CE1	2:F:209:ARG:HB2	2.49	0.48
4:I:3:ARG:NH1	4:I:59:ASP:OD2	2.47	0.48
3:A:255:GLN:HB3	3:A:273:ARG:NH2	2.29	0.48
1:E:123:LEU:HD11	1:E:135:LEU:HB2	1.95	0.48
2:G:47:ILE:HG13	2:G:57:LYS:HG3	1.95	0.48
2:G:207:HIS:CE1	2:G:209:ARG:HB2	2.48	0.48
1:E:123:LEU:HB2	1:E:133:VAL:HG13	1.96	0.48
3:H:59:TYR:O	3:H:63:GLU:HG2	2.14	0.47
1:D:25:SER:OG	1:D:73:ARG:NH2	2.47	0.47
4:I:5:PRO:HB3	4:I:30:PHE:HB3	1.95	0.47
2:G:242:ARG:HG2	2:G:243:ALA:H	1.80	0.47
3:H:78:LEU:HG	3:H:95:LEU:HD12	1.97	0.47
4:I:38:ASP:HB3	4:I:45:ARG:HG2	1.97	0.47
3:H:8:PHE:CE2	3:H:98:MET:HG3	2.50	0.46
3:A:219:ARG:N	3:A:222:GLU:O	2.35	0.46
1:E:140:ASP:OD1	1:E:143:THR:OG1	2.18	0.46
3:A:215:LEU:HD23	3:A:261:VAL:HB	1.97	0.46
2:G:154:HIS:HB3	2:G:215:TYR:HB2	1.98	0.45
4:B:48:LYS:HB2	1:E:127:LYS:NZ	2.32	0.45
2:G:120:VAL:HG12	2:G:230:PRO:HB2	1.99	0.45
2:G:170:VAL:HG22	2:G:194:LEU:HD13	1.99	0.45
2:G:185:ASP:N	2:G:185:ASP:OD1	2.50	0.45
2:F:21:LEU:HD22	2:F:109:THR:HG21	1.99	0.45
3:A:22:PHE:H	3:A:38:SER:HB3	1.82	0.44
3:A:127:ASN:HD22	3:A:132:SER:HB2	1.82	0.44
3:A:203:CYS:HB2	3:A:217:TRP:CZ2	2.53	0.44
3:A:5:MET:HB2	3:A:168:LEU:HD13	1.98	0.44
2:G:110:ARG:HD3	2:G:154:HIS:NE2	2.32	0.43
3:H:14:ARG:HB2	3:H:17:ARG:HB2	1.99	0.43
4:I:42:ASN:HA	4:I:77:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:LEU:HG	3:A:249:VAL:HG11	2.01	0.43
4:B:19:LYS:O	4:B:72:PRO:HD2	2.18	0.43
2:F:140:LYS:HE2	2:F:140:LYS:HB3	1.87	0.43
1:E:123:LEU:HD23	2:G:130:PRO:HA	2.00	0.43
4:B:96:ASP:HB3	4:B:99:MET:HB2	2.01	0.43
4:B:5:PRO:HB2	4:B:27:VAL:HG23	2.01	0.42
1:D:12:LEU:HD21	1:D:20:LEU:HD22	2.00	0.42
3:H:203:CYS:HB2	3:H:217:TRP:CZ2	2.55	0.42
1:E:101:PHE:CD2	2:G:43:LEU:HD23	2.55	0.42
3:H:99:TYR:CZ	5:J:3:VAL:HG12	2.54	0.42
1:D:32:TYR:O	1:D:53:SER:HB2	2.19	0.42
3:H:197:HIS:ND1	3:H:198:GLU:HG3	2.34	0.42
3:A:59:TYR:O	3:A:63:GLU:HG2	2.20	0.42
4:B:36:GLU:HB3	4:B:83:ASN:HB3	2.01	0.42
2:F:185:ASP:N	2:F:185:ASP:OD1	2.52	0.42
2:F:32:VAL:HG21	2:F:74:SER:HB2	2.00	0.42
3:H:31:THR:HG23	3:H:239:ARG:HD3	2.01	0.42
2:G:207:HIS:HB2	2:G:240:TRP:CZ3	2.56	0.41
3:H:223:ASP:OD1	3:H:223:ASP:N	2.54	0.41
4:B:25:CYS:HB2	4:B:39:LEU:HD21	2.02	0.41
1:D:123:LEU:HD11	1:D:135:LEU:HB2	2.02	0.40
2:F:12:ILE:HD12	2:F:152:PRO:HG2	2.03	0.40
1:E:174:VAL:HG23	2:G:193:ARG:HE	1.86	0.40
1:E:8:ILE:HD12	6:E:301:NAG:H83	2.03	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	D	199/204 (98%)	192 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	F	236/241 (98%)	227 (96%)	9 (4%)	0	100	100
2	G	238/241 (99%)	228 (96%)	10 (4%)	0	100	100
3	A	274/278 (99%)	264 (96%)	10 (4%)	0	100	100
3	H	274/278 (99%)	265 (97%)	9 (3%)	0	100	100
4	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
4	I	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
5	C	7/9 (78%)	7 (100%)	0	0	100	100
5	J	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1629/1664 (98%)	1574 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	D	179/182 (98%)	174 (97%)	5 (3%)	43	73
1	E	179/182 (98%)	179 (100%)	0	100	100
2	F	207/211 (98%)	200 (97%)	7 (3%)	37	66
2	G	208/211 (99%)	201 (97%)	7 (3%)	37	66
3	A	235/237 (99%)	226 (96%)	9 (4%)	33	62
3	H	235/237 (99%)	227 (97%)	8 (3%)	37	66
4	B	94/95 (99%)	91 (97%)	3 (3%)	39	68
4	I	94/95 (99%)	93 (99%)	1 (1%)	73	90
5	C	8/8 (100%)	8 (100%)	0	100	100
5	J	8/8 (100%)	8 (100%)	0	100	100
All	All	1447/1466 (99%)	1407 (97%)	40 (3%)	43	73

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	LYS
1	D	5	VAL
1	D	14	VAL
1	D	73	ARG
1	D	124	ARG
2	F	9	LYS
2	F	17	GLN
2	F	171	CYS
2	F	202	GLN
2	F	206	ASN
2	F	219	GLU
2	F	220	ASN
3	A	35	ARG
3	A	38	SER
3	A	106	ASP
3	A	134	THR
3	A	196	ASP
3	A	223	ASP
3	A	226	GLN
3	A	254	GLU
3	A	261	VAL
4	B	19	LYS
4	B	48	LYS
4	B	70	PHE
2	G	134	GLU
2	G	138	THR
2	G	171	CYS
2	G	180	GLN
2	G	202	GLN
2	G	206	ASN
2	G	242	ARG
3	H	14	ARG
3	H	35	ARG
3	H	106	ASP
3	H	163	GLU
3	H	248	VAL
3	H	254	GLU
3	H	255	GLN
3	H	256	ARG
4	I	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	171	ASN

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](#)

13 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	$\# Z > 2$
6	NAG	E	302	1	14,14,15	0.27	0	17,19,21	0.47	0
6	NAG	D	302	1	14,14,15	0.24	0	17,19,21	0.42	0
7	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.06	0
8	GOL	G	303	-	5,5,5	0.90	0	5,5,5	1.16	1 (20%)
6	NAG	F	301	2	14,14,15	0.27	0	17,19,21	0.37	0
6	NAG	G	301	2	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	E	301	1	14,14,15	0.30	0	17,19,21	0.41	0
7	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.05	0
8	GOL	G	302	-	5,5,5	0.87	0	5,5,5	1.00	0
6	NAG	D	301	1	14,14,15	0.37	0	17,19,21	0.41	0
7	SO4	E	304	-	4,4,4	0.14	0	6,6,6	0.06	0
8	GOL	E	303	-	5,5,5	0.90	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	G	304	-	4,4,4	0.13	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	302	1	-	2/6/23/26	0/1/1/1
6	NAG	D	302	1	-	4/6/23/26	0/1/1/1
8	GOL	G	303	-	-	0/4/4/4	-
6	NAG	F	301	2	-	0/6/23/26	0/1/1/1
6	NAG	G	301	2	-	2/6/23/26	0/1/1/1
6	NAG	E	301	1	-	2/6/23/26	0/1/1/1
8	GOL	G	302	-	-	2/4/4/4	-
6	NAG	D	301	1	-	2/6/23/26	0/1/1/1
8	GOL	E	303	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	303	GOL	C3-C2-C1	-2.11	103.50	111.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	302	NAG	O5-C5-C6-O6
6	D	301	NAG	O5-C5-C6-O6
6	G	301	NAG	O5-C5-C6-O6
6	D	301	NAG	C4-C5-C6-O6
6	E	302	NAG	C4-C5-C6-O6
6	D	302	NAG	C8-C7-N2-C2
6	D	302	NAG	O7-C7-N2-C2
6	E	301	NAG	C8-C7-N2-C2
6	E	301	NAG	O7-C7-N2-C2
6	D	302	NAG	O5-C5-C6-O6
6	G	301	NAG	C4-C5-C6-O6
6	D	302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	G	302	GOL	O2-C2-C3-O3
8	G	302	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	301	NAG	1	0
8	G	302	GOL	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 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	D	201/204 (98%)	0.35	19 (9%) 8 6	50, 96, 151, 189	0
1	E	201/204 (98%)	-0.16	6 (2%) 50 51	41, 68, 125, 168	0
2	F	238/241 (98%)	-0.11	6 (2%) 57 59	42, 73, 137, 202	0
2	G	240/241 (99%)	-0.12	6 (2%) 57 59	39, 78, 127, 189	0
3	A	276/278 (99%)	-0.32	3 (1%) 80 82	40, 63, 112, 145	0
3	H	276/278 (99%)	-0.37	2 (0%) 87 89	39, 59, 115, 142	0
4	B	100/100 (100%)	-0.20	0 100 100	47, 76, 116, 146	0
4	I	99/100 (99%)	-0.07	2 (2%) 65 67	46, 76, 118, 133	0
5	C	9/9 (100%)	-0.41	0 100 100	45, 51, 62, 68	0
5	J	9/9 (100%)	-0.39	0 100 100	44, 49, 52, 55	0
All	All	1649/1664 (99%)	-0.15	44 (2%) 54 55	39, 70, 130, 202	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	124	ARG	5.5
1	D	202	PRO	4.5
3	A	227	ASP	3.9
1	D	114	GLN	3.9
2	G	205	ARG	3.7
2	G	243	ALA	3.7
1	D	129	SER	3.7
1	D	144	ASN	3.6
1	D	124	ARG	3.6
1	D	126	SER	3.5
1	D	128	SER	3.5
1	D	199	PHE	3.3
2	G	177	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	132	GLU	3.2
1	E	180	SER	3.1
1	D	193	ILE	3.0
1	D	172	SER	2.9
1	E	195	GLU	2.8
2	F	241	GLY	2.8
1	D	119	ALA	2.8
1	D	192	ILE	2.8
2	F	182	ALA	2.7
1	D	127	LYS	2.7
2	G	185	ASP	2.7
1	D	167	ASP	2.7
1	D	173	ALA	2.5
2	F	135	ILE	2.5
1	D	174	VAL	2.4
3	H	197	HIS	2.3
1	E	114	GLN	2.3
1	D	132	SER	2.3
1	D	151	SER	2.3
2	G	178	LYS	2.3
2	F	200	PHE	2.3
2	G	242	ARG	2.2
1	E	193	ILE	2.2
4	I	44	GLU	2.2
1	E	42	GLY	2.1
3	A	198	GLU	2.1
4	I	99	MET	2.1
1	D	131	LYS	2.0
3	A	197	HIS	2.0
3	H	42	SER	2.0
2	F	128	PHE	2.0

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 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, 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	B-factors(Å ²)	Q<0.9
8	GOL	G	303	6/6	0.83	0.20	78,81,89,89	0
6	NAG	E	302	14/15	0.86	0.25	70,83,100,101	0
6	NAG	D	302	14/15	0.86	0.30	103,110,113,116	0
6	NAG	D	301	14/15	0.89	0.23	77,94,106,108	0
6	NAG	E	301	14/15	0.91	0.18	81,89,107,109	0
8	GOL	E	303	6/6	0.93	0.16	56,76,81,82	0
6	NAG	F	301	14/15	0.93	0.20	61,77,85,88	0
6	NAG	G	301	14/15	0.94	0.14	72,81,91,92	0
7	SO4	H	301	5/5	0.94	0.15	87,108,124,125	0
8	GOL	G	302	6/6	0.95	0.33	54,62,74,75	0
7	SO4	F	302	5/5	0.96	0.14	84,91,110,121	0
7	SO4	G	304	5/5	0.96	0.13	71,95,101,122	0
7	SO4	E	304	5/5	0.97	0.10	72,79,94,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.