



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 AM UTC

PDB ID : 3SE3 / pdb_00003se3
Title : human IFNa2-IFNAR ternary complex
Authors : Thomas, C.; Garcia, K.C.
Deposited on : 2011-06-10
Resolution : 4.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

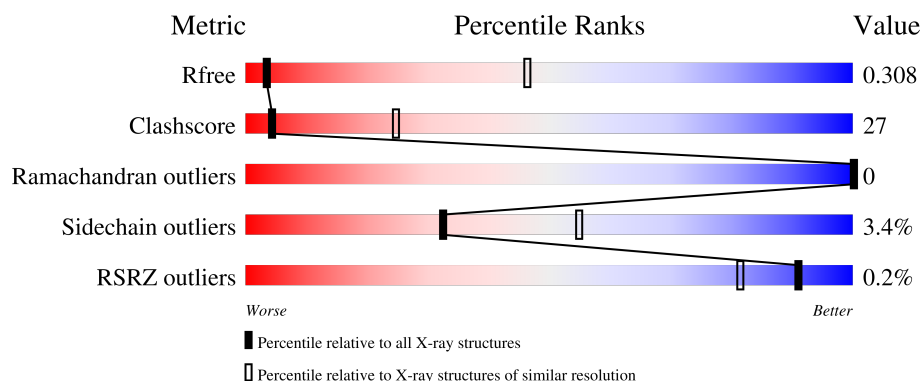
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 ≥ 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	414	
2	B	166	
3	C	199	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4462 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 Interferon alpha/beta receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2025	1297	336	383	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	cloning artifact	UNP P17181
A	-3	ASP	-	cloning artifact	UNP P17181
A	-2	LEU	-	cloning artifact	UNP P17181
A	-1	GLY	-	cloning artifact	UNP P17181
A	0	SER	-	cloning artifact	UNP P17181

- Molecule 2 is a protein called Interferon alpha 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			1006	647	160	192	7			

There are 3 discrepancies between the modelled and reference sequences:

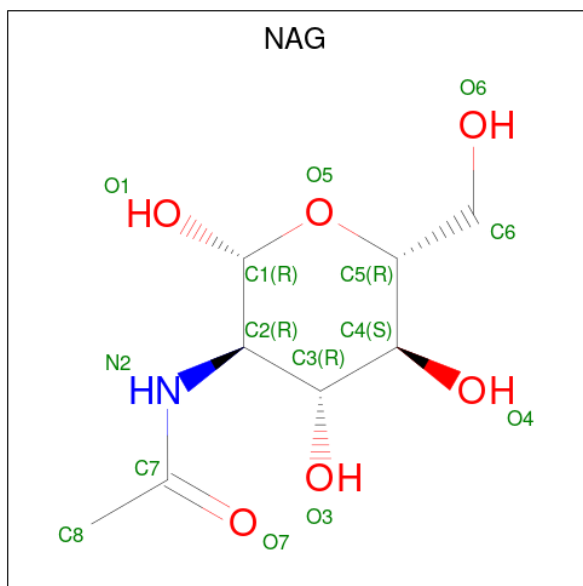
Chain	Residue	Modelled	Actual	Comment	Reference
B	57	TYR	HIS	engineered mutation	UNP Q86UP4
B	58	ASN	GLU	engineered mutation	UNP Q86UP4
B	61	SER	GLN	engineered mutation	UNP Q86UP4

- Molecule 3 is a protein called Interferon alpha/beta receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1417	912	226	270	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

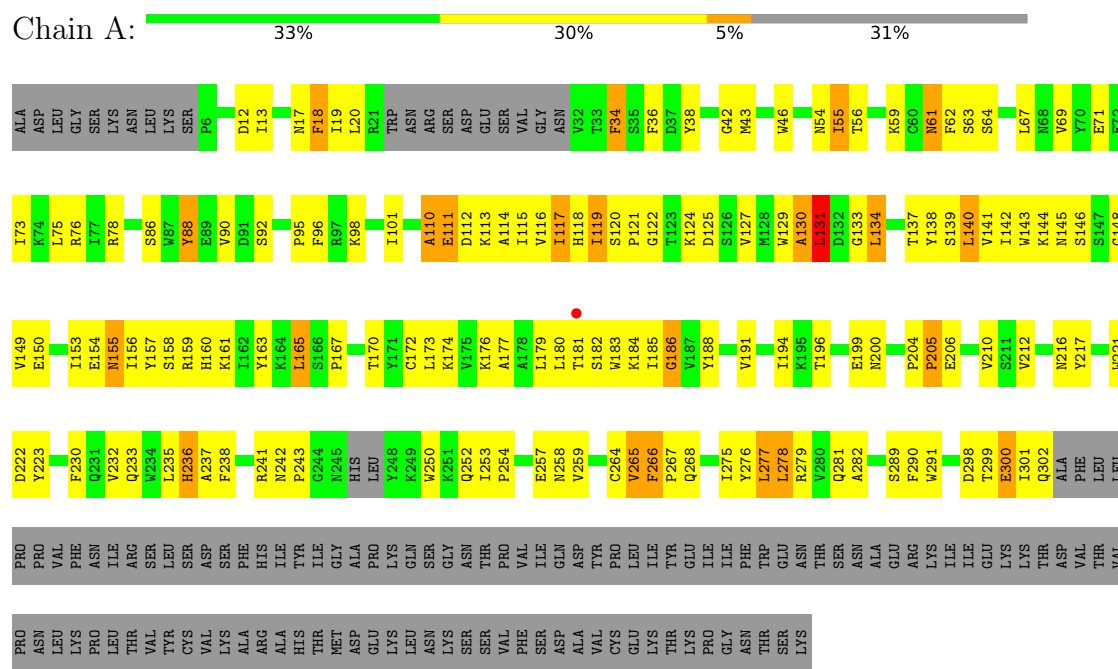


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

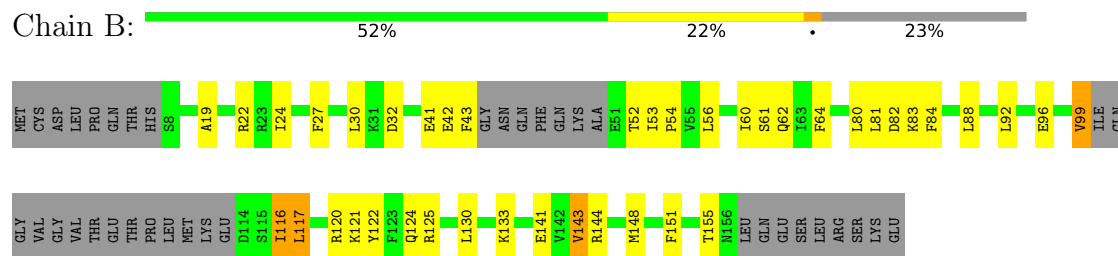
3 Residue-property plots

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.

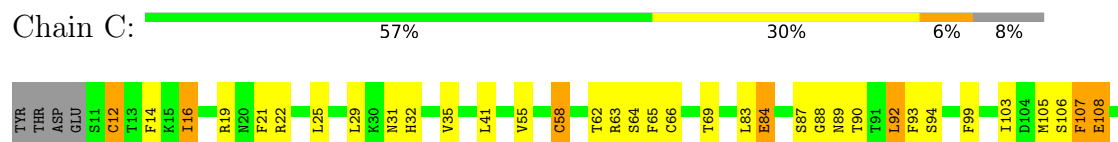
• Molecule 1: Interferon alpha/beta receptor 1



• Molecule 2: Interferon alpha 2b



• Molecule 3: Interferon alpha/beta receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.37Å 93.37Å 401.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 4.00 46.78 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.78-4.00) 99.8 (46.78-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.311 0.250 , 0.308	Depositor DCC
R_{free} test set	477 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	137.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 191.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4462	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.66	0/2075	1.44	43/2854 (1.5%)
2	B	0.65	0/1026	1.06	5/1389 (0.4%)
3	C	0.63	0/1452	1.39	25/1980 (1.3%)
All	All	0.65	0/4553	1.35	73/6223 (1.2%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	N-CA-C	12.64	126.62	111.33
1	A	69	VAL	N-CA-CB	-11.17	97.42	112.28
1	A	122	GLY	N-CA-C	-10.99	97.66	112.82
3	C	108	GLU	CA-C-N	10.84	127.46	119.66
3	C	108	GLU	C-N-CA	10.84	127.46	119.66
3	C	65	PHE	CA-C-N	-10.21	108.59	122.99
3	C	65	PHE	C-N-CA	-10.21	108.59	122.99
3	C	89	ASN	N-CA-C	-10.07	101.17	113.15
1	A	266	PHE	CA-C-N	9.43	129.26	120.21
1	A	266	PHE	C-N-CA	9.43	129.26	120.21
1	A	13	ILE	N-CA-C	9.25	121.44	108.12
1	A	206	GLU	N-CA-C	8.72	124.28	111.02
3	C	191	GLN	N-CA-CB	8.05	121.77	110.17
1	A	210	VAL	N-CA-C	7.68	119.66	108.53
3	C	35	VAL	CA-C-N	7.36	129.04	119.84
3	C	35	VAL	C-N-CA	7.36	129.04	119.84
3	C	181	VAL	N-CA-C	7.26	118.94	108.48
1	A	117	ILE	N-CA-C	7.15	118.17	107.80
1	A	19	ILE	N-CA-C	7.15	119.25	107.24
1	A	253	ILE	CA-C-N	6.93	126.18	118.97
1	A	253	ILE	C-N-CA	6.93	126.18	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	103	ILE	CB-CA-C	-6.91	104.67	111.30
3	C	151	VAL	N-CA-C	6.90	117.83	108.17
1	A	111	GLU	N-CA-C	6.76	119.22	109.14
3	C	64	SER	CA-C-N	-6.75	110.77	122.37
3	C	64	SER	C-N-CA	-6.75	110.77	122.37
1	A	133	GLY	N-CA-C	6.54	120.58	112.73
1	A	110	ALA	N-CA-C	6.40	120.31	110.20
3	C	31	ASN	N-CA-C	6.23	119.69	111.28
1	A	223	TYR	N-CA-C	-6.21	99.58	109.76
1	A	13	ILE	CB-CA-C	-6.17	101.32	110.33
1	A	69	VAL	N-CA-C	-6.12	106.35	112.17
1	A	140	LEU	N-CA-C	6.04	118.14	109.14
1	A	61	ASN	N-CA-C	5.99	119.40	109.46
2	B	151	PHE	N-CA-C	5.98	117.80	111.28
1	A	204	PRO	N-CA-C	5.97	116.97	110.58
3	C	121	ILE	N-CA-C	5.89	116.36	108.11
2	B	143	VAL	N-CA-C	5.89	116.67	110.72
1	A	119	ILE	N-CA-C	5.89	117.24	108.46
1	A	180	LEU	N-CA-C	-5.87	105.22	112.38
1	A	36	PHE	N-CA-C	5.86	118.44	108.02
1	A	119	ILE	CB-CA-C	-5.84	101.51	110.50
2	B	96	GLU	N-CA-C	-5.81	104.63	110.97
3	C	176	ASN	N-CA-C	5.76	119.61	112.24
1	A	116	VAL	N-CA-C	5.71	116.16	108.17
1	A	205	PRO	N-CA-C	-5.67	102.20	111.21
2	B	117	LEU	N-CA-C	-5.64	105.13	111.28
3	C	107	PHE	N-CA-C	5.62	118.21	107.75
1	A	38	TYR	N-CA-C	5.62	117.93	109.23
3	C	92	LEU	N-CA-C	5.59	120.23	113.41
1	A	278	LEU	N-CA-C	5.58	118.65	109.72
3	C	120	HIS	N-CA-C	5.56	116.72	108.60
3	C	139	LEU	N-CA-C	5.50	118.00	110.24
3	C	12	CYS	N-CA-C	5.49	118.35	109.40
1	A	258	ASN	N-CA-C	5.46	119.23	112.24
1	A	265	VAL	N-CA-C	5.35	116.56	108.96
1	A	88	TYR	N-CA-C	5.32	118.09	107.62
1	A	115	ILE	N-CA-C	5.31	116.37	108.46
1	A	131	LEU	N-CA-C	5.30	117.14	111.36
2	B	99	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	153	ILE	CB-CA-C	-5.28	105.22	111.09
3	C	16	ILE	N-CA-C	5.28	115.46	107.75
1	A	34	PHE	N-CA-C	5.26	118.17	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ALA	N-CA-C	5.24	117.04	109.07
1	A	42	GLY	N-CA-C	-5.22	107.84	115.72
1	A	155	ASN	N-CA-C	5.19	118.75	111.74
3	C	84	GLU	CA-C-N	-5.17	117.63	121.61
3	C	84	GLU	C-N-CA	-5.17	117.63	121.61
1	A	186	GLY	N-CA-C	5.12	121.55	112.64
1	A	18	PHE	N-CA-CB	-5.11	102.47	110.69
1	A	236	HIS	N-CA-C	-5.10	102.84	110.23
1	A	130	ALA	CB-CA-C	-5.09	110.69	116.54
3	C	188	SER	N-CA-C	-5.08	101.48	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2025	0	1671	130	0
2	B	1006	0	931	37	0
3	C	1417	0	1327	61	0
4	A	14	0	13	4	0
All	All	4462	0	3942	224	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 27.

All (224) 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)
1:A:145:ASN:HD21	4:A:410:NAG:C1	1.39	1.35
3:C:29:LEU:HB3	3:C:32:HIS:HD2	1.22	1.05
1:A:118:HIS:HA	1:A:159:ARG:HG2	1.45	0.98
3:C:19:ARG:HG2	3:C:108:GLU:HG3	1.46	0.96
1:A:18:PHE:CE1	1:A:62:PHE:CE2	2.56	0.93
1:A:18:PHE:O	1:A:59:LYS:HA	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HA	1:A:129:TRP:HZ2	1.38	0.88
1:A:111:GLU:O	1:A:196:THR:HB	1.74	0.88
1:A:101:ILE:HA	1:A:129:TRP:CZ2	2.07	0.88
1:A:174:LYS:HE3	1:A:188:TYR:CG	2.10	0.86
3:C:29:LEU:HB3	3:C:32:HIS:CD2	2.13	0.81
1:A:217:TYR:CE1	1:A:268:GLN:HA	2.16	0.80
2:B:116:ILE:HG13	2:B:117:LEU:N	1.98	0.78
3:C:22:ARG:HE	3:C:69:THR:CB	1.98	0.77
1:A:46:TRP:HB3	1:A:76:ARG:NH2	2.00	0.75
3:C:88:GLY:C	3:C:90:THR:H	1.95	0.74
1:A:18:PHE:CZ	1:A:62:PHE:CE2	2.76	0.72
1:A:176:LYS:HD3	1:A:188:TYR:CZ	2.23	0.72
1:A:63:SER:O	1:A:64:SER:HB3	1.88	0.72
1:A:120:SER:HB2	1:A:121:PRO:HD2	1.71	0.71
1:A:173:LEU:HD12	1:A:173:LEU:C	2.16	0.70
1:A:216:ASN:HA	1:A:267:PRO:HA	1.74	0.70
1:A:145:ASN:CG	4:A:410:NAG:C1	2.64	0.70
3:C:173:LEU:CB	3:C:203:LEU:HD11	2.22	0.70
3:C:170:ILE:HG22	3:C:173:LEU:HD21	1.74	0.70
2:B:81:LEU:O	2:B:84:PHE:HB3	1.92	0.69
1:A:55:ILE:HD12	1:A:56:THR:H	1.58	0.68
1:A:259:VAL:HG11	1:A:264:CYS:HB3	1.75	0.67
2:B:41:GLU:CD	2:B:41:GLU:H	2.02	0.67
2:B:122:TYR:HA	2:B:125:ARG:CZ	2.25	0.67
1:A:43:MET:SD	1:A:46:TRP:CZ2	2.88	0.66
3:C:173:LEU:HB2	3:C:203:LEU:HD11	1.77	0.66
3:C:105:MET:HG3	3:C:106:SER:N	2.11	0.66
1:A:176:LYS:HB3	1:A:188:TYR:CD1	2.31	0.65
3:C:117:PHE:C	3:C:204:PRO:HD2	2.22	0.64
1:A:217:TYR:HB2	1:A:266:PHE:O	1.97	0.64
3:C:25:LEU:O	3:C:66:CYS:N	2.25	0.64
3:C:84:GLU:HG2	3:C:94:SER:HB3	1.79	0.64
2:B:19:ALA:HB2	2:B:148:MET:HE1	1.79	0.64
1:A:254:PRO:O	1:A:257:GLU:HG2	1.97	0.63
3:C:146:GLN:HB3	3:C:180:CYS:O	1.99	0.63
1:A:205:PRO:HB3	1:A:221:TRP:CD1	2.33	0.63
3:C:22:ARG:HE	3:C:69:THR:HB	1.64	0.62
1:A:150:GLU:O	1:A:150:GLU:HG3	1.99	0.62
3:C:124:MET:SD	3:C:165:ASN:HB3	2.40	0.62
3:C:21:PHE:O	3:C:22:ARG:HD2	2.00	0.61
3:C:177:THR:C	3:C:202:LEU:HD13	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:O	1:A:62:PHE:CD1	2.52	0.61
2:B:130:LEU:HD11	2:B:143:VAL:HG21	1.81	0.61
3:C:139:LEU:HD23	3:C:187:HIS:HA	1.83	0.61
1:A:140:LEU:HD23	1:A:156:ILE:HD13	1.83	0.60
3:C:41:LEU:O	3:C:55:VAL:HG12	2.01	0.60
1:A:298:ASP:OD1	1:A:298:ASP:O	2.20	0.60
3:C:184:TYR:CE1	3:C:195:LYS:NZ	2.68	0.59
1:A:124:LYS:O	1:A:125:ASP:HB2	2.00	0.59
1:A:17:ASN:OD1	1:A:61:ASN:HB2	2.03	0.58
1:A:174:LYS:HE3	1:A:188:TYR:CD1	2.39	0.58
1:A:46:TRP:CB	1:A:76:ARG:NH2	2.67	0.58
3:C:25:LEU:HD23	3:C:41:LEU:HD11	1.84	0.58
1:A:182:SER:C	1:A:184:LYS:H	2.10	0.57
1:A:182:SER:C	1:A:184:LYS:N	2.61	0.57
1:A:145:ASN:HD21	4:A:410:NAG:C2	2.11	0.57
1:A:18:PHE:CE1	1:A:62:PHE:CZ	2.92	0.57
1:A:143:TRP:HD1	1:A:144:LYS:O	1.88	0.57
1:A:221:TRP:HZ2	1:A:230:PHE:CD2	2.23	0.57
3:C:87:SER:H	3:C:92:LEU:CD1	2.19	0.56
1:A:12:ASP:HA	1:A:98:LYS:HD3	1.88	0.55
1:A:142:ILE:HG13	1:A:172:CYS:O	2.06	0.55
1:A:160:HIS:CD2	1:A:161:LYS:H	2.24	0.55
1:A:119:ILE:HG21	1:A:138:TYR:CE1	2.41	0.55
2:B:121:LYS:O	2:B:124:GLN:HB3	2.07	0.55
3:C:87:SER:N	3:C:92:LEU:CD1	2.70	0.54
3:C:88:GLY:C	3:C:90:THR:N	2.62	0.54
3:C:120:HIS:HA	3:C:173:LEU:HD12	1.88	0.54
3:C:173:LEU:HB3	3:C:203:LEU:HD11	1.87	0.54
1:A:110:ALA:HB2	1:A:194:ILE:CD1	2.38	0.54
1:A:230:PHE:HA	1:A:281:GLN:O	2.07	0.54
1:A:179:LEU:C	1:A:181:THR:H	2.14	0.54
1:A:163:TYR:O	1:A:165:LEU:HD13	2.07	0.54
1:A:160:HIS:CD2	1:A:161:LYS:N	2.76	0.54
3:C:12:CYS:HB3	3:C:29:LEU:HD23	1.90	0.54
1:A:46:TRP:CB	1:A:76:ARG:HH22	2.21	0.54
1:A:157:TYR:CD1	1:A:241:ARG:HG3	2.43	0.54
1:A:176:LYS:HD3	1:A:188:TYR:CE2	2.42	0.54
1:A:160:HIS:HD2	1:A:161:LYS:H	1.55	0.53
1:A:75:LEU:HB2	1:A:90:VAL:HB	1.91	0.53
1:A:139:SER:CB	1:A:154:GLU:HA	2.38	0.53
1:A:179:LEU:C	1:A:181:THR:N	2.64	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:CB	1:A:275:ILE:HG22	2.38	0.53
3:C:12:CYS:HB3	3:C:29:LEU:CD2	2.39	0.53
3:C:55:VAL:HG13	3:C:58:CYS:HB2	1.89	0.53
3:C:117:PHE:O	3:C:204:PRO:HD2	2.08	0.53
1:A:113:LYS:O	1:A:165:LEU:HB2	2.09	0.52
3:C:62:THR:HG23	3:C:63:ARG:N	2.25	0.52
1:A:221:TRP:CZ2	1:A:230:PHE:CG	2.98	0.52
2:B:52:THR:HG23	2:B:56:LEU:HD13	1.92	0.52
1:A:182:SER:O	1:A:184:LYS:N	2.43	0.52
1:A:137:THR:CG2	1:A:155:ASN:HA	2.41	0.51
1:A:184:LYS:C	1:A:185:ILE:HG13	2.35	0.51
1:A:299:THR:O	1:A:300:GLU:OE1	2.29	0.51
1:A:143:TRP:HB3	1:A:150:GLU:HA	1.92	0.51
3:C:156:PRO:HG3	3:C:168:TYR:CD1	2.46	0.51
1:A:134:LEU:HD12	2:B:64:PHE:CD2	2.46	0.50
1:A:134:LEU:HD21	1:A:242:ASN:HA	1.91	0.50
1:A:129:TRP:HA	1:A:129:TRP:HE3	1.76	0.50
2:B:27:PHE:HD2	2:B:30:LEU:HD12	1.75	0.50
1:A:73:ILE:O	1:A:92:SER:HA	2.10	0.50
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.46	0.50
1:A:134:LEU:O	1:A:134:LEU:HD13	2.12	0.50
1:A:86:SER:HB2	1:A:88:TYR:CE2	2.47	0.50
1:A:145:ASN:OD1	4:A:410:NAG:C1	2.58	0.50
1:A:221:TRP:HZ2	1:A:230:PHE:CG	2.29	0.50
3:C:62:THR:CG2	3:C:63:ARG:N	2.75	0.49
1:A:138:TYR:HB2	1:A:156:ILE:CG1	2.43	0.49
1:A:157:TYR:HD1	1:A:241:ARG:HG3	1.78	0.49
2:B:122:TYR:HA	2:B:125:ARG:NH2	2.28	0.49
2:B:155:THR:HG22	2:B:155:THR:O	2.12	0.49
1:A:173:LEU:HD12	1:A:173:LEU:O	2.11	0.49
2:B:80:LEU:O	2:B:81:LEU:C	2.53	0.49
1:A:279:ARG:HG3	1:A:291:TRP:CZ3	2.48	0.48
1:A:129:TRP:O	1:A:130:ALA:C	2.53	0.48
2:B:60:ILE:HG23	2:B:88:LEU:HD22	1.95	0.48
1:A:259:VAL:HG11	1:A:264:CYS:CB	2.43	0.48
2:B:42:GLU:HB2	2:B:43:PHE:CE2	2.49	0.48
3:C:151:VAL:HG23	3:C:151:VAL:O	2.13	0.48
3:C:83:LEU:O	3:C:94:SER:HA	2.14	0.48
1:A:111:GLU:HG2	1:A:290:PHE:CE1	2.48	0.48
1:A:145:ASN:HB2	1:A:170:THR:HG22	1.96	0.48
3:C:184:TYR:HB3	3:C:195:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:N	1:A:20:LEU:HD23	2.28	0.48
3:C:25:LEU:HD23	3:C:41:LEU:CD1	2.44	0.48
1:A:142:ILE:HG12	1:A:143:TRP:N	2.28	0.47
3:C:22:ARG:NE	3:C:69:THR:HB	2.29	0.47
1:A:238:PHE:CD1	1:A:238:PHE:C	2.92	0.47
1:A:101:ILE:HB	1:A:186:GLY:HA3	1.94	0.47
1:A:140:LEU:HD12	1:A:140:LEU:C	2.39	0.47
1:A:158:SER:CB	1:A:243:PRO:HB3	2.45	0.47
3:C:87:SER:N	3:C:92:LEU:HD11	2.29	0.47
3:C:126:LYS:HE2	3:C:126:LYS:HB3	1.52	0.47
1:A:143:TRP:CD1	1:A:148:GLY:HA2	2.50	0.47
3:C:140:SER:OG	3:C:155:LYS:NZ	2.47	0.47
1:A:138:TYR:HB2	1:A:156:ILE:HG13	1.95	0.47
2:B:32:ASP:OD1	2:B:133:LYS:NZ	2.35	0.47
3:C:107:PHE:CD1	3:C:139:LEU:HD11	2.50	0.47
2:B:121:LYS:HD2	2:B:124:GLN:HB3	1.96	0.46
1:A:63:SER:O	1:A:64:SER:CB	2.57	0.46
1:A:282:ALA:O	1:A:289:SER:N	2.46	0.46
2:B:53:ILE:N	2:B:54:PRO:CD	2.77	0.46
3:C:127:PHE:HB2	3:C:164:GLY:O	2.15	0.46
3:C:92:LEU:O	3:C:93:PHE:HB3	2.15	0.46
1:A:124:LYS:O	1:A:125:ASP:CB	2.64	0.46
1:A:145:ASN:HB2	1:A:170:THR:O	2.16	0.46
2:B:43:PHE:CD2	2:B:43:PHE:N	2.84	0.46
1:A:237:ALA:HB3	1:A:275:ILE:HG22	1.97	0.46
1:A:131:LEU:HB2	2:B:62:GLN:OE1	2.16	0.45
3:C:107:PHE:CE1	3:C:139:LEU:HD11	2.52	0.45
1:A:232:VAL:O	1:A:252:GLN:HG3	2.16	0.45
1:A:110:ALA:HB2	1:A:194:ILE:HD13	1.98	0.45
1:A:142:ILE:O	1:A:150:GLU:HA	2.16	0.45
3:C:21:PHE:O	3:C:22:ARG:CD	2.64	0.45
1:A:61:ASN:C	1:A:61:ASN:OD1	2.60	0.45
3:C:87:SER:H	3:C:92:LEU:HD12	1.81	0.45
2:B:22:ARG:HG3	2:B:144:ARG:NH2	2.31	0.45
3:C:121:ILE:HG13	3:C:173:LEU:CD1	2.47	0.45
3:C:174:ILE:HG22	3:C:175:PRO:O	2.17	0.45
2:B:82:ASP:O	2:B:83:LYS:C	2.60	0.45
1:A:236:HIS:CE1	1:A:276:TYR:CE1	3.05	0.44
2:B:27:PHE:CD2	2:B:30:LEU:HD12	2.53	0.44
1:A:167:PRO:HG2	1:A:199:GLU:HB2	1.99	0.44
1:A:235:LEU:HB2	1:A:250:TRP:CE3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:ARG:HG3	2:B:144:ARG:HH21	1.81	0.44
3:C:120:HIS:C	3:C:173:LEU:HD12	2.43	0.44
3:C:156:PRO:HG3	3:C:168:TYR:CE1	2.53	0.44
1:A:112:ASP:CB	1:A:199:GLU:HA	2.48	0.44
1:A:212:VAL:HG23	1:A:216:ASN:O	2.18	0.44
2:B:122:TYR:HB2	2:B:125:ARG:NH2	2.33	0.44
3:C:147:SER:HB3	3:C:179:TYR:CD1	2.53	0.44
2:B:24:ILE:CG1	2:B:141:GLU:HG3	2.48	0.44
1:A:182:SER:O	1:A:183:TRP:C	2.61	0.43
1:A:301:ILE:O	1:A:302:GLN:CB	2.65	0.43
1:A:71:GLU:O	1:A:95:PRO:HD2	2.19	0.43
1:A:150:GLU:O	1:A:150:GLU:CG	2.65	0.43
2:B:60:ILE:C	2:B:62:GLN:N	2.73	0.43
2:B:130:LEU:HD23	2:B:130:LEU:HA	1.86	0.43
3:C:87:SER:H	3:C:92:LEU:HD11	1.83	0.43
1:A:173:LEU:O	1:A:191:VAL:HA	2.18	0.43
1:A:143:TRP:CD1	1:A:144:LYS:O	2.69	0.43
1:A:277:LEU:C	1:A:278:LEU:HG	2.42	0.43
1:A:140:LEU:CD2	1:A:156:ILE:HD13	2.49	0.43
1:A:142:ILE:CG1	1:A:143:TRP:N	2.82	0.43
1:A:101:ILE:HG21	1:A:177:ALA:HB3	2.01	0.43
1:A:119:ILE:HG21	1:A:138:TYR:CD1	2.54	0.43
3:C:22:ARG:NE	3:C:69:THR:CB	2.74	0.42
1:A:176:LYS:HB3	1:A:188:TYR:CE1	2.54	0.42
2:B:60:ILE:CG2	2:B:92:LEU:HD21	2.49	0.42
1:A:18:PHE:CZ	1:A:62:PHE:CD2	3.07	0.42
1:A:86:SER:HB2	1:A:88:TYR:HE2	1.84	0.42
1:A:200:ASN:CB	1:A:290:PHE:CD2	3.03	0.42
1:A:139:SER:HB2	1:A:154:GLU:HA	2.01	0.42
3:C:16:ILE:HG23	3:C:16:ILE:O	2.20	0.42
1:A:117:ILE:HG22	1:A:119:ILE:HG13	2.02	0.42
2:B:22:ARG:HB2	2:B:144:ARG:NH2	2.35	0.41
3:C:25:LEU:CD2	3:C:41:LEU:HD11	2.48	0.41
2:B:116:ILE:HG13	2:B:117:LEU:H	1.82	0.41
3:C:142:VAL:HG11	3:C:184:TYR:OH	2.20	0.41
3:C:14:PHE:HB3	3:C:99:PHE:HZ	1.85	0.41
1:A:96:PHE:CE2	2:B:116:ILE:HD11	2.55	0.41
2:B:60:ILE:O	2:B:61:SER:C	2.63	0.41
3:C:203:LEU:HA	3:C:204:PRO:HD3	1.74	0.41
1:A:101:ILE:HA	1:A:129:TRP:CH2	2.50	0.41
1:A:276:TYR:CD2	1:A:276:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:OE1	1:A:279:ARG:NH2	2.46	0.41
2:B:22:ARG:CG	2:B:144:ARG:NH2	2.84	0.41
1:A:43:MET:HE2	1:A:43:MET:HB3	1.84	0.41
3:C:105:MET:HG3	3:C:106:SER:H	1.80	0.41
1:A:34:PHE:O	1:A:54:ASN:N	2.54	0.41
1:A:119:ILE:CG2	1:A:138:TYR:CE1	3.04	0.41
3:C:202:LEU:N	3:C:202:LEU:CD2	2.84	0.41
1:A:34:PHE:HA	1:A:78:ARG:O	2.21	0.40
1:A:141:VAL:CG1	1:A:150:GLU:HB2	2.51	0.40
2:B:41:GLU:CD	2:B:41:GLU:N	2.77	0.40
2:B:116:ILE:O	2:B:120:ARG:N	2.50	0.40
1:A:96:PHE:HE2	2:B:116:ILE:HD11	1.86	0.40
1:A:155:ASN:O	1:A:155:ASN:CG	2.62	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	279/414 (67%)	259 (93%)	20 (7%)	0	100	100
2	B	122/166 (74%)	118 (97%)	4 (3%)	0	100	100
3	C	177/199 (89%)	168 (95%)	9 (5%)	0	100	100
All	All	578/779 (74%)	545 (94%)	33 (6%)	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	A	174/382 (46%)	163 (94%)	11 (6%)	16	41
2	B	105/153 (69%)	103 (98%)	2 (2%)	50	67
3	C	158/189 (84%)	156 (99%)	2 (1%)	61	72
All	All	437/724 (60%)	422 (97%)	15 (3%)	32	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	127	VAL
1	A	131	LEU
1	A	134	LEU
1	A	146	SER
1	A	149	VAL
1	A	165	LEU
1	A	222	ASP
1	A	265	VAL
1	A	277	LEU
1	A	300	GLU
2	B	99	VAL
2	B	116	ILE
3	C	58	CYS
3	C	150	ILE

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	145	ASN
1	A	160	HIS
2	B	34	HIS
2	B	90	GLN
2	B	124	GLN
3	C	20	ASN
3	C	32	HIS
3	C	97	HIS
3	C	122	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	A	410	1	14,14,15	0.60	0	17,19,21	1.07	2 (11%)

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	A	410	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	410	NAG	C1-O5-C5	-3.16	107.95	112.19
4	A	410	NAG	O5-C1-C2	-2.11	108.03	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	410	NAG	4	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	285/414 (68%)	-0.14	1 (0%) 88 75	92, 168, 270, 345	0
2	B	128/166 (77%)	-0.40	0 100 100	93, 132, 168, 198	0
3	C	183/199 (91%)	-0.30	0 100 100	104, 153, 208, 264	0
All	All	596/779 (76%)	-0.25	1 (0%) 91 81	92, 154, 246, 345	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	2.3

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 oligosaccharides 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
4	NAG	A	410	14/15	0.32	0.10	159,208,221,228	0

6.5 Other polymers [i](#)

There are no such residues in this entry.