



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:24 AM UTC

PDB ID : 3D5O / pdb_00003d5o
Title : Structural recognition and functional activation of FcrR by innate pentraxins
Authors : Lu, J.; Marnell, L.L.; Marjon, K.D.; Mold, C.; Du Clos, T.W.; Sun, P.D.
Deposited on : 2008-05-16
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

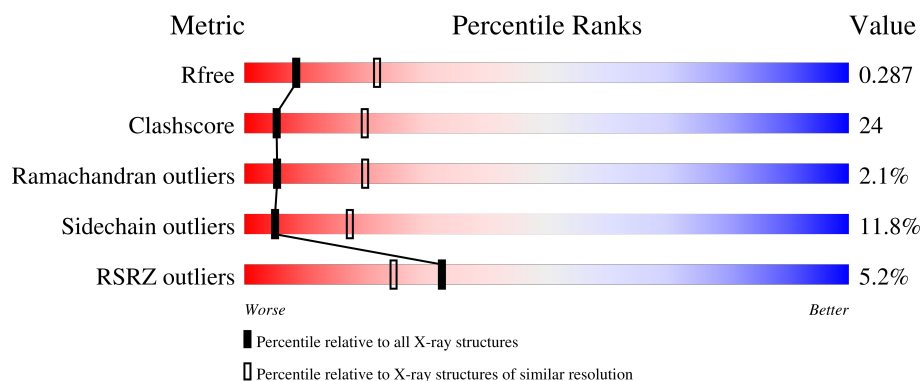
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	204	4% 59% 35% 5%
1	B	204	61% 32% 5%
1	C	204	4% 56% 36% 7%
1	D	204	5% 51% 40% 9%
1	E	204	3% 48% 42% 9%

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Mol	Chain	Length	Quality of chain
2	F	177	14% 46% 37% 12% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9655 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 Serum amyloid P-component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1638	1064	268	303	3			
1	B	204	Total	C	N	O	S	0	0	0
			1642	1067	269	303	3			
1	C	204	Total	C	N	O	S	0	0	0
			1624	1057	263	301	3			
1	D	204	Total	C	N	O	S	0	0	0
			1620	1054	262	301	3			
1	E	204	Total	C	N	O	S	0	0	0
			1631	1060	265	303	3			

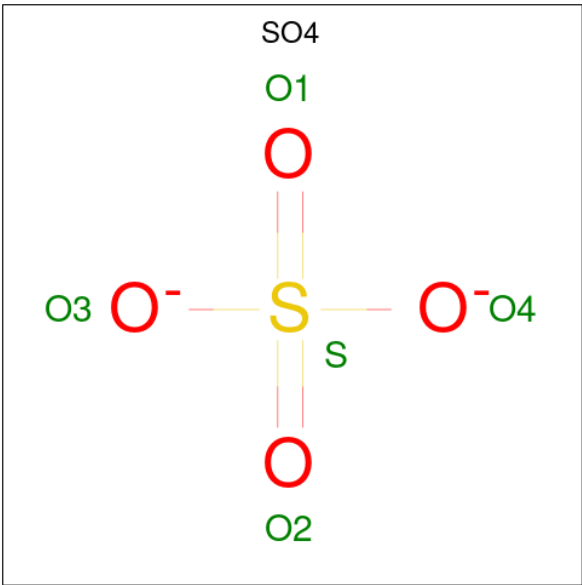
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor II-a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	171	Total	C	N	O	S	0	0	0
			1313	829	226	253	5			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	131	ARG	HIS	SEE REMARK 999	UNP P12318
F	172	HIS	-	expression tag	UNP P12318
F	173	HIS	-	expression tag	UNP P12318
F	174	HIS	-	expression tag	UNP P12318
F	175	HIS	-	expression tag	UNP P12318
F	176	HIS	-	expression tag	UNP P12318
F	177	HIS	-	expression tag	UNP P12318

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



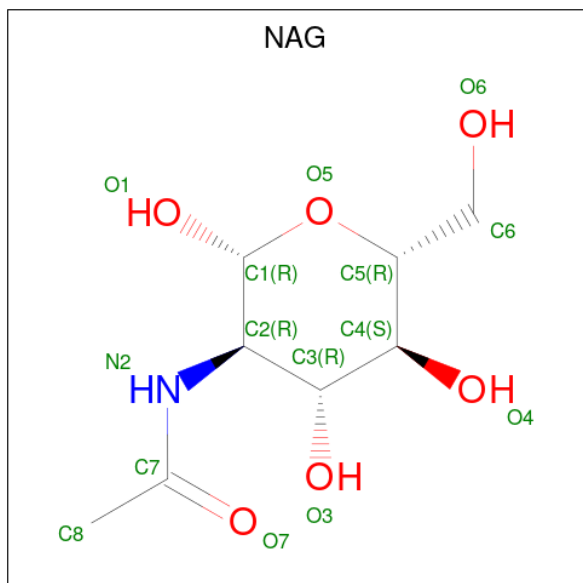
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

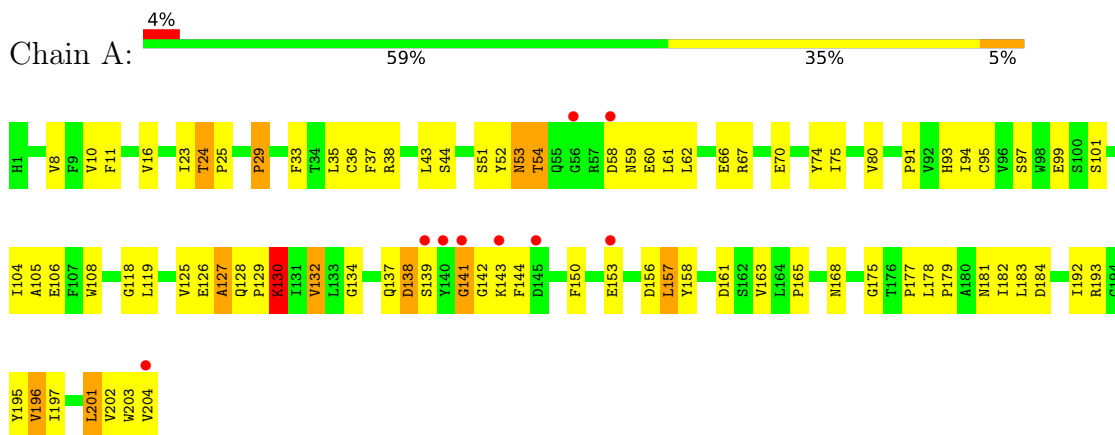
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	13	Total	O	0	0
			13	13		
6	C	6	Total	O	0	0
			6	6		
6	D	3	Total	O	0	0
			3	3		
6	E	1	Total	O	0	0
			1	1		
6	F	5	Total	O	0	0
			5	5		

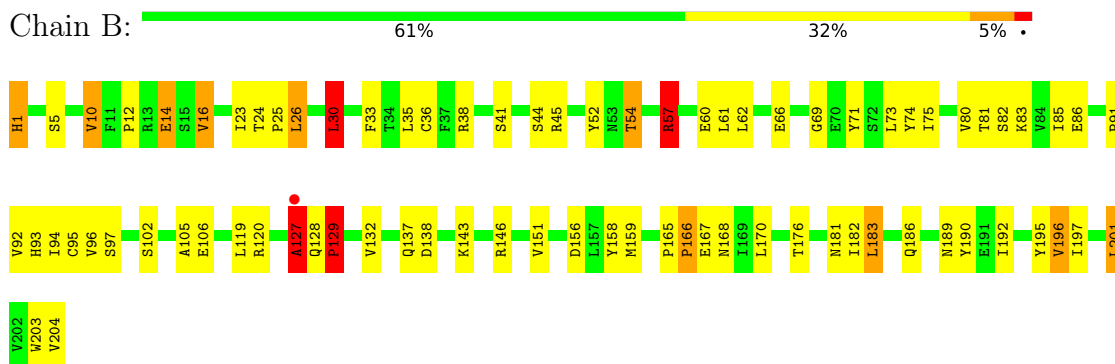
3 Residue-property plots [i](#)

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.

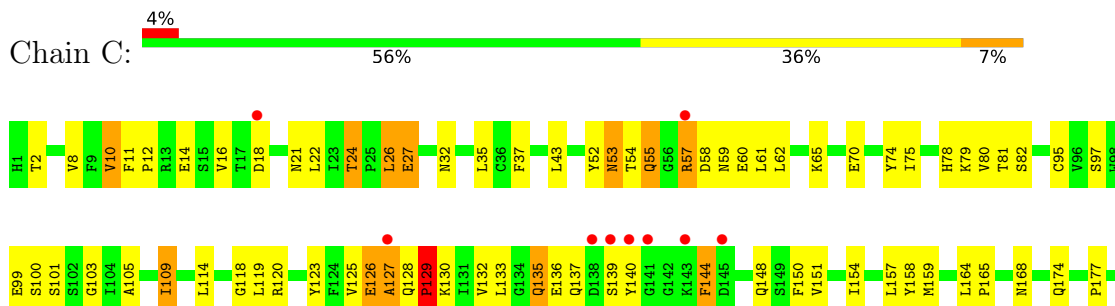
- Molecule 1: Serum amyloid P-component



- Molecule 1: Serum amyloid P-component

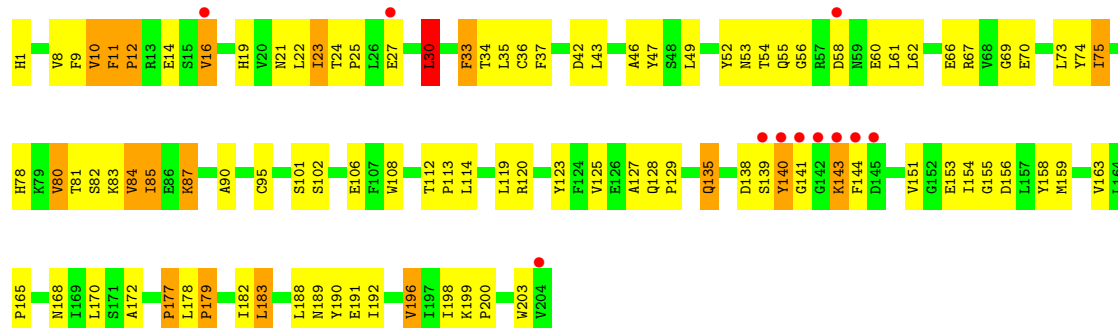


- Molecule 1: Serum amyloid P-component

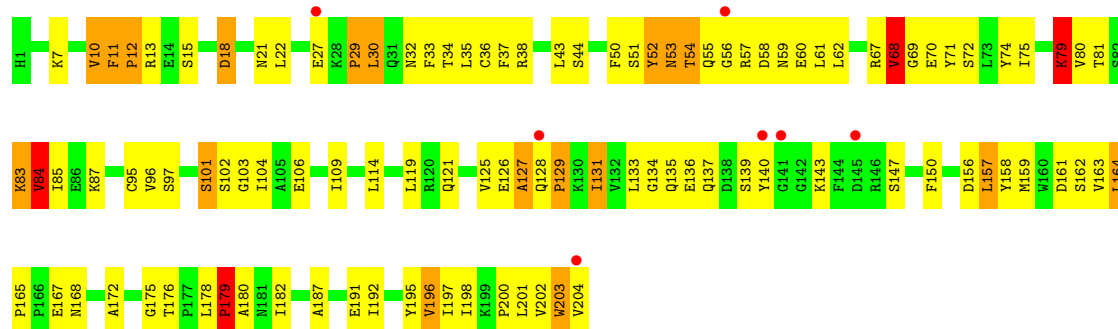




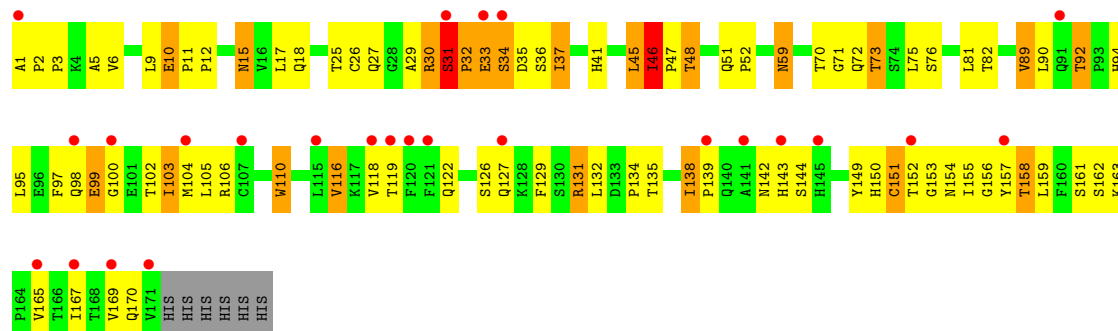
• Molecule 1: Serum amyloid P-component



• Molecule 1: Serum amyloid P-component



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor II-a



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.20Å 143.48Å 161.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 97.6 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.279 0.218 , 0.287	Depositor DCC
R_{free} test set	1471 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9655	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, SO4, 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	0.53	0/1685	1.05	6/2293 (0.3%)
1	B	0.56	0/1689	1.08	15/2297 (0.7%)
1	C	0.51	0/1671	1.06	7/2274 (0.3%)
1	D	0.51	0/1667	1.03	8/2270 (0.4%)
1	E	0.45	0/1678	1.08	17/2284 (0.7%)
2	F	0.51	0/1351	1.19	21/1851 (1.1%)
All	All	0.51	0/9741	1.08	74/13269 (0.6%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	143	HIS	N-CA-C	-10.26	100.76	113.28
1	E	127	ALA	N-CA-C	9.86	125.11	112.89
1	A	127	ALA	N-CA-C	9.23	124.85	113.50
1	A	129	PRO	N-CA-C	8.18	124.04	111.19
1	A	11	PHE	CA-C-N	8.14	127.78	119.56
1	A	11	PHE	C-N-CA	8.14	127.78	119.56
2	F	32	PRO	N-CA-C	8.11	123.93	111.19
1	E	129	PRO	N-CA-C	7.74	123.69	111.38
1	E	69	GLY	N-CA-C	-7.66	104.63	115.43
1	D	11	PHE	CA-C-N	7.48	127.64	119.87
1	D	11	PHE	C-N-CA	7.48	127.64	119.87
2	F	33	GLU	N-CA-C	-7.47	97.36	108.34
1	C	100	SER	N-CA-C	-7.32	103.97	113.12
2	F	46	ILE	CA-C-N	7.31	127.65	119.32
2	F	46	ILE	C-N-CA	7.31	127.65	119.32
1	B	127	ALA	N-CA-C	7.19	126.11	110.80
2	F	2	PRO	N-CA-C	7.19	119.47	110.70
1	C	11	PHE	CA-C-N	7.17	128.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	PHE	C-N-CA	7.17	128.81	119.84
1	D	30	LEU	N-CA-C	6.84	120.09	109.07
2	F	1	ALA	CA-C-N	6.59	127.17	120.38
2	F	1	ALA	C-N-CA	6.59	127.17	120.38
1	E	53	ASN	N-CA-C	6.57	118.20	108.60
1	C	18	ASP	N-CA-C	6.56	119.87	110.10
1	E	128	GLN	CA-C-N	6.48	126.40	119.85
1	E	128	GLN	C-N-CA	6.48	126.40	119.85
2	F	31	SER	CA-C-N	-6.46	113.30	119.76
2	F	31	SER	C-N-CA	-6.46	113.30	119.76
1	E	11	PHE	CA-C-N	6.41	126.90	119.47
1	E	11	PHE	C-N-CA	6.41	126.90	119.47
1	B	26	LEU	N-CA-C	6.38	118.56	108.67
1	E	84	VAL	CB-CA-C	-6.29	103.06	111.80
1	C	129	PRO	N-CA-C	6.25	125.35	112.47
1	B	57	ARG	N-CA-C	6.24	119.41	109.24
1	A	104	ILE	N-CA-C	6.24	117.12	108.89
1	E	30	LEU	N-CA-C	6.20	119.58	109.59
1	C	132	VAL	N-CA-C	6.12	116.73	108.17
2	F	12	PRO	N-CA-C	6.08	121.49	114.20
1	E	172	ALA	N-CA-C	-5.96	104.91	111.82
1	B	129	PRO	N-CA-C	5.93	121.67	111.77
2	F	33	GLU	N-CA-CB	5.93	117.10	111.59
2	F	46	ILE	N-CA-C	-5.89	96.15	108.88
1	B	120	ARG	N-CA-C	5.78	119.61	111.52
1	C	127	ALA	N-CA-C	5.73	121.17	113.72
1	B	195	TYR	N-CA-C	5.72	118.08	108.23
2	F	118	VAL	N-CA-C	5.72	116.83	108.53
1	E	164	LEU	CA-C-N	5.69	123.76	119.66
1	E	164	LEU	C-N-CA	5.69	123.76	119.66
1	D	11	PHE	N-CA-C	-5.64	97.53	108.59
1	E	85	ILE	N-CA-C	-5.64	99.60	108.23
1	A	130	LYS	N-CA-C	-5.62	98.19	108.02
2	F	95	LEU	N-CA-C	-5.58	106.39	113.43
1	B	128	GLN	CA-C-N	5.58	126.74	120.66
1	B	128	GLN	C-N-CA	5.58	126.74	120.66
1	E	79	LYS	N-CA-C	5.58	118.78	110.14
1	E	12	PRO	N-CA-C	5.55	121.86	113.81
1	D	172	ALA	N-CA-C	-5.53	105.34	111.36
1	B	181	ASN	N-CA-C	5.52	119.86	113.18
1	D	12	PRO	N-CA-C	5.52	120.82	114.03
2	F	138	ILE	CA-C-N	5.51	126.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	138	ILE	C-N-CA	5.51	126.72	119.84
1	B	30	LEU	N-CA-C	5.50	118.58	109.46
1	B	12	PRO	N-CA-C	5.49	120.78	114.03
1	B	14	GLU	N-CA-C	-5.35	101.26	109.76
2	F	163	LYS	CA-C-N	5.33	125.64	119.93
2	F	163	LYS	C-N-CA	5.33	125.64	119.93
1	D	90	ALA	N-CA-C	5.32	112.92	108.13
1	B	23	ILE	N-CA-C	5.17	115.76	108.36
2	F	135	THR	N-CA-C	5.17	117.91	109.59
1	D	106	GLU	N-CA-C	5.15	117.46	108.76
2	F	37	ILE	N-CA-C	5.13	115.87	108.48
1	B	85	ILE	N-CA-C	-5.11	102.91	109.30
1	E	147	SER	N-CA-C	-5.08	107.03	113.18
1	B	132	VAL	N-CA-C	5.07	116.02	108.46

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	1638	0	1600	80	0
1	B	1642	0	1611	52	0
1	C	1624	0	1583	88	0
1	D	1620	0	1572	81	0
1	E	1631	0	1588	91	0
2	F	1313	0	1228	70	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
3	E	15	0	0	1	0
3	F	5	0	0	0	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	13	0	0
4	E	14	0	13	0	0
5	F	6	0	8	3	0
6	A	3	0	0	1	0
6	B	13	0	0	0	0
6	C	6	0	0	1	0
6	D	3	0	0	0	0
6	E	1	0	0	0	0
6	F	5	0	0	0	0
All	All	9655	0	9255	457	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 24.

All (457) 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:C:54:THR:CG2	1:C:57:ARG:HG3	1.55	1.35
1:C:54:THR:CG2	1:C:57:ARG:CG	2.15	1.23
2:F:30:ARG:NH2	2:F:72:GLN:HB2	1.64	1.13
1:C:54:THR:HG21	1:C:57:ARG:HG3	1.07	1.03
2:F:30:ARG:HH22	2:F:72:GLN:HB2	0.88	1.03
1:E:192:ILE:HG23	1:E:196:VAL:HG13	1.41	1.02
2:F:37:ILE:HD12	2:F:52:PRO:HA	1.43	1.01
1:A:130:LYS:HG2	1:A:137:GLN:NE2	1.75	1.00
1:D:52:TYR:HB3	1:D:61:LEU:HB2	1.45	0.98
1:D:192:ILE:HG23	1:D:196:VAL:HG13	1.47	0.97
1:C:53:ASN:ND2	1:C:137:GLN:HG3	1.82	0.95
1:E:52:TYR:HB3	1:E:61:LEU:HB2	1.47	0.95
1:A:130:LYS:NZ	1:A:132:VAL:CG1	2.31	0.94
1:D:53:ASN:OD1	1:D:58:ASP:HA	1.68	0.93
2:F:70:THR:HB	2:F:73:THR:OG1	1.68	0.93
1:A:99:GLU:HG3	1:A:163:VAL:HG21	1.50	0.92
1:C:80:VAL:HG13	1:C:119:LEU:HD13	1.52	0.91
1:E:38:ARG:HD2	1:E:156:ASP:OD2	1.70	0.90
1:E:34:THR:HG21	1:E:164:LEU:H	1.36	0.90
1:D:47:TYR:HE1	1:D:49:LEU:HD21	1.35	0.89
1:C:54:THR:HG21	1:C:57:ARG:CG	1.91	0.89
1:A:130:LYS:NZ	1:A:132:VAL:HG11	1.88	0.88
1:E:75:ILE:HD11	1:E:119:LEU:HG	1.53	0.88
2:F:103:ILE:HG23	2:F:138:ILE:HB	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HG23	1:A:196:VAL:HG13	1.56	0.87
1:D:54:THR:HG22	1:D:55:GLN:H	1.39	0.86
1:C:54:THR:CG2	1:C:57:ARG:HG2	2.05	0.86
1:C:37:PHE:HB3	1:C:157:LEU:HD12	1.58	0.85
2:F:30:ARG:HH22	2:F:72:GLN:CB	1.82	0.85
2:F:45:LEU:O	2:F:47:PRO:HD3	1.77	0.84
2:F:59:ASN:C	2:F:59:ASN:HD22	1.85	0.84
1:A:130:LYS:HZ1	1:A:132:VAL:HG11	1.43	0.83
1:B:24:THR:HG23	1:B:182:ILE:O	1.79	0.83
1:C:54:THR:HG23	1:C:57:ARG:HG2	1.59	0.83
1:E:62:LEU:HB3	1:E:74:TYR:HB2	1.59	0.83
1:A:165:PRO:HD2	1:A:168:ASN:HD22	1.42	0.83
1:D:14:GLU:HG2	1:D:151:VAL:HG21	1.60	0.82
1:E:27:GLU:O	1:E:127:ALA:HB1	1.79	0.82
1:A:130:LYS:HZ3	1:A:132:VAL:CG1	1.92	0.81
1:B:127:ALA:O	1:B:129:PRO:HD3	1.80	0.81
1:C:55:GLN:HE21	1:C:128:GLN:HB2	1.44	0.81
1:A:157:LEU:HD12	1:A:158:TYR:N	1.95	0.80
1:C:54:THR:HG22	1:C:57:ARG:CG	2.10	0.80
1:A:130:LYS:HG2	1:A:137:GLN:HE22	1.44	0.79
1:A:137:GLN:HG2	1:A:141:GLY:HA2	1.63	0.79
1:E:134:GLY:HA2	1:E:150:PHE:HB3	1.64	0.78
1:D:21:ASN:HB2	1:D:191:GLU:HB2	1.64	0.78
1:C:24:THR:HG23	1:C:182:ILE:O	1.83	0.78
2:F:157:TYR:O	2:F:158:THR:HG23	1.82	0.78
2:F:151:CYS:H	2:F:162:SER:HB3	1.46	0.78
1:C:54:THR:HG22	1:C:57:ARG:HG3	1.62	0.78
1:B:41:SER:HB2	1:B:151:VAL:O	1.84	0.77
2:F:31:SER:HB3	2:F:32:PRO:HD2	1.66	0.77
1:B:1:HIS:HB3	1:B:189:ASN:ND2	2.00	0.76
1:D:54:THR:HG22	1:D:55:GLN:N	2.01	0.76
1:D:84:VAL:HG13	1:D:114:LEU:HD21	1.68	0.75
1:E:21:ASN:HB2	1:E:191:GLU:HB2	1.68	0.75
2:F:17:LEU:HD21	2:F:89:VAL:HG23	1.68	0.75
1:A:24:THR:HG21	1:A:182:ILE:HG23	1.68	0.75
1:D:75:ILE:HG22	1:D:119:LEU:HD11	1.68	0.75
1:A:192:ILE:CG2	1:A:196:VAL:HG13	2.17	0.75
1:D:192:ILE:HG23	1:D:196:VAL:CG1	2.17	0.75
1:D:108:TRP:CZ3	1:D:113:PRO:HG3	2.22	0.74
1:B:165:PRO:HD2	1:B:168:ASN:HD22	1.52	0.74
1:C:52:TYR:HB3	1:C:61:LEU:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HE21	1:A:141:GLY:HA2	1.54	0.73
1:D:24:THR:HG23	1:D:182:ILE:O	1.89	0.72
1:C:204:VAL:CG1	2:F:156:GLY:HA3	2.19	0.72
1:D:75:ILE:HG23	1:D:120:ARG:HG3	1.72	0.72
1:B:167:GLU:H	1:B:167:GLU:CD	1.98	0.71
1:A:52:TYR:HB3	1:A:61:LEU:HB3	1.72	0.71
1:A:130:LYS:HZ1	1:A:132:VAL:CG1	1.99	0.71
1:B:192:ILE:HG23	1:B:196:VAL:HG13	1.71	0.71
1:E:139:SER:HB3	1:E:143:LYS:HD2	1.73	0.71
1:C:10:VAL:O	1:C:12:PRO:HD3	1.90	0.70
1:E:60:GLU:OE2	1:E:126:GLU:HG2	1.92	0.70
2:F:34:SER:HB2	5:F:179:GOL:O3	1.92	0.70
1:C:137:GLN:NE2	1:C:144:PHE:HE1	1.89	0.69
1:E:161:ASP:HB3	1:E:182:ILE:HD11	1.74	0.69
1:C:192:ILE:HG23	1:C:196:VAL:HG13	1.73	0.69
2:F:119:THR:CG2	2:F:129:PHE:HD1	2.07	0.68
1:E:11:PHE:CE1	1:E:134:GLY:HA3	2.28	0.68
1:E:29:PRO:HD3	1:E:127:ALA:HB2	1.75	0.68
1:C:52:TYR:O	1:C:60:GLU:HB3	1.94	0.67
1:C:55:GLN:NE2	1:C:128:GLN:H	1.92	0.67
1:A:130:LYS:CG	1:A:137:GLN:NE2	2.57	0.67
2:F:15:ASN:ND2	2:F:90:LEU:O	2.27	0.67
1:A:137:GLN:HE21	1:A:141:GLY:CA	2.08	0.67
1:D:1:HIS:HA	1:D:188:LEU:O	1.94	0.66
1:E:102:SER:HB2	1:E:104:ILE:HG12	1.75	0.66
1:A:54:THR:HG21	1:A:126:GLU:HB3	1.77	0.66
1:B:52:TYR:HB3	1:B:61:LEU:HB2	1.77	0.66
1:E:35:LEU:O	1:E:95:CYS:HA	1.96	0.66
2:F:35:ASP:O	2:F:36:SER:HB2	1.96	0.66
1:E:159:MET:O	1:E:180:ALA:HB1	1.97	0.65
1:E:50:PHE:O	1:E:62:LEU:HD12	1.97	0.65
1:E:53:ASN:HD21	1:E:137:GLN:HB3	1.61	0.64
1:E:165:PRO:HD2	1:E:168:ASN:HD22	1.61	0.64
1:C:27:GLU:O	1:C:127:ALA:HB1	1.97	0.64
1:C:165:PRO:HD2	1:C:168:ASN:ND2	2.13	0.64
1:C:174:GLN:HA	1:C:174:GLN:NE2	2.13	0.64
1:B:75:ILE:HG13	1:B:119:LEU:HD21	1.79	0.64
1:D:54:THR:CG2	1:D:55:GLN:H	2.11	0.64
1:B:62:LEU:HB3	1:B:74:TYR:HB2	1.79	0.63
1:C:75:ILE:HG22	1:C:119:LEU:HD11	1.78	0.63
1:A:53:ASN:HD21	1:A:59:ASN:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HG13	1:D:114:LEU:CD2	2.29	0.63
1:B:57:ARG:N	1:B:57:ARG:HD2	2.14	0.62
1:C:159:MET:O	1:C:182:ILE:HB	1.99	0.62
1:C:137:GLN:HE21	1:C:144:PHE:HE1	1.45	0.62
1:D:8:VAL:HG11	1:D:153:GLU:HB3	1.80	0.62
1:D:80:VAL:HG21	1:D:119:LEU:HD22	1.80	0.62
1:A:130:LYS:CG	1:A:137:GLN:HE22	2.13	0.62
1:E:192:ILE:HG23	1:E:196:VAL:CG1	2.25	0.62
1:E:35:LEU:HD11	1:E:157:LEU:HD11	1.82	0.62
2:F:152:THR:HG22	2:F:161:SER:HB3	1.80	0.62
1:A:67:ARG:NH1	1:A:70:GLU:OE2	2.32	0.62
2:F:30:ARG:HD3	2:F:70:THR:HG21	1.82	0.62
1:A:118:GLY:HA3	1:E:12:PRO:HB2	1.82	0.62
1:D:52:TYR:O	1:D:60:GLU:HB3	1.99	0.62
1:E:101:SER:O	1:E:121:GLN:HG3	2.00	0.62
1:C:74:TYR:CZ	1:C:79:LYS:HD2	2.35	0.61
1:C:135:GLN:HE21	1:C:136:GLU:H	1.46	0.61
2:F:18:GLN:HB2	2:F:110:TRP:HZ3	1.65	0.61
4:A:208:NAG:H82	4:A:208:NAG:O3	2.00	0.61
1:E:34:THR:HG21	1:E:164:LEU:N	2.11	0.61
1:A:157:LEU:HD12	1:A:157:LEU:C	2.25	0.61
1:C:204:VAL:HG11	2:F:156:GLY:HA3	1.81	0.61
1:E:10:VAL:O	1:E:12:PRO:HD3	2.01	0.61
1:E:192:ILE:CG2	1:E:196:VAL:HG13	2.26	0.61
1:E:54:THR:HA	1:E:140:TYR:CE1	2.36	0.60
1:D:165:PRO:HD2	1:D:168:ASN:HD22	1.67	0.60
1:E:54:THR:HA	1:E:140:TYR:HE1	1.67	0.60
1:B:176:THR:HG22	1:D:25:PRO:HB3	1.83	0.60
1:A:130:LYS:HG2	1:A:137:GLN:HE21	1.66	0.60
1:B:1:HIS:HB3	1:B:189:ASN:HD21	1.64	0.60
1:D:47:TYR:CE1	1:D:49:LEU:HD21	2.27	0.60
2:F:75:LEU:HD13	2:F:76:SER:O	2.02	0.60
1:E:67:ARG:O	1:E:68:VAL:HG23	2.01	0.60
2:F:26:CYS:HB3	2:F:37:ILE:HD13	1.82	0.59
2:F:31:SER:CB	2:F:32:PRO:HD2	2.32	0.59
1:D:8:VAL:HG13	1:D:154:ILE:O	2.02	0.59
1:E:70:GLU:HG2	1:E:83:LYS:HD2	1.85	0.59
1:A:62:LEU:HD23	1:A:74:TYR:CD1	2.38	0.58
2:F:119:THR:HG23	2:F:129:PHE:HD1	1.68	0.58
1:C:140:TYR:HB3	6:C:210:HOH:O	2.03	0.58
2:F:30:ARG:HG2	2:F:31:SER:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD11	1:A:157:LEU:HD11	1.86	0.58
2:F:153:GLY:O	2:F:159:LEU:HA	2.04	0.58
2:F:106:ARG:HA	2:F:134:PRO:O	2.04	0.58
1:C:8:VAL:HG11	1:C:201:LEU:HD13	1.86	0.57
1:E:51:SER:OG	1:E:136:GLU:HA	2.04	0.57
2:F:97:PHE:O	2:F:169:VAL:HA	2.04	0.57
1:D:47:TYR:HE1	1:D:49:LEU:CD2	2.14	0.57
1:D:54:THR:HA	1:D:140:TYR:HE1	1.70	0.57
2:F:92:THR:HG21	2:F:167:ILE:HD11	1.86	0.57
1:A:130:LYS:NZ	1:A:132:VAL:HG12	2.19	0.57
1:C:21:ASN:HB2	1:C:191:GLU:HG3	1.85	0.57
1:C:35:LEU:O	1:C:95:CYS:HA	2.05	0.57
1:A:8:VAL:HG13	1:A:201:LEU:HB2	1.86	0.57
1:D:33:PHE:CD1	1:D:33:PHE:C	2.82	0.57
1:C:150:PHE:CE2	1:C:154:ILE:HG12	2.39	0.57
1:A:197:ILE:N	1:A:197:ILE:HD12	2.19	0.57
2:F:41:HIS:HB2	2:F:46:ILE:HD11	1.86	0.56
1:C:60:GLU:OE1	1:C:60:GLU:HA	2.05	0.56
1:B:24:THR:HG21	1:B:182:ILE:HG23	1.86	0.56
2:F:45:LEU:HD13	2:F:47:PRO:CA	2.36	0.56
1:E:54:THR:C	1:E:140:TYR:HD1	2.13	0.56
1:D:19:HIS:HB3	1:D:135:GLN:HG3	1.87	0.56
1:C:55:GLN:CD	1:C:55:GLN:H	2.12	0.56
1:C:137:GLN:NE2	1:C:144:PHE:CE1	2.71	0.56
1:A:161:ASP:CG	1:A:181:ASN:HD21	2.14	0.55
1:D:139:SER:O	1:D:140:TYR:HB2	2.06	0.55
1:A:36:CYS:HA	1:A:94:ILE:O	2.06	0.55
1:A:29:PRO:CD	1:A:127:ALA:HB2	2.36	0.55
1:A:192:ILE:HG23	1:A:196:VAL:CG1	2.33	0.55
1:C:62:LEU:HB3	1:C:74:TYR:HB2	1.89	0.55
1:C:192:ILE:CG2	1:C:196:VAL:HG13	2.37	0.55
1:E:34:THR:CG2	1:E:164:LEU:H	2.14	0.55
1:C:197:ILE:HD12	1:C:197:ILE:N	2.22	0.55
1:D:75:ILE:O	1:D:75:ILE:HD13	2.07	0.55
1:A:23:ILE:N	1:A:23:ILE:HD12	2.22	0.54
1:C:24:THR:HG21	1:C:182:ILE:HG23	1.89	0.54
1:E:54:THR:C	1:E:140:TYR:CD1	2.86	0.54
1:A:53:ASN:OD1	1:A:58:ASP:HA	2.08	0.54
1:E:203:TRP:CD1	1:E:203:TRP:H	2.24	0.54
2:F:29:ALA:N	2:F:30:ARG:HD2	2.22	0.54
1:C:54:THR:HG22	1:C:57:ARG:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:VAL:CG1	1:C:119:LEU:HD13	2.32	0.54
1:E:53:ASN:ND2	1:E:137:GLN:HB3	2.22	0.54
2:F:90:LEU:HD12	2:F:150:HIS:HA	1.90	0.54
1:D:85:ILE:HD12	1:D:85:ILE:O	2.07	0.54
2:F:10:GLU:HA	2:F:11:PRO:C	2.32	0.54
1:A:58:ASP:O	1:A:59:ASN:HB2	2.07	0.54
1:E:55:GLN:N	1:E:140:TYR:CD1	2.76	0.53
2:F:15:ASN:OD1	2:F:15:ASN:N	2.41	0.53
1:B:57:ARG:HD2	1:B:57:ARG:H	1.73	0.53
2:F:119:THR:HG23	2:F:129:PHE:CD1	2.44	0.53
1:A:196:VAL:C	1:A:197:ILE:HD12	2.33	0.53
2:F:29:ALA:H	2:F:30:ARG:HD2	1.73	0.53
1:D:84:VAL:CG1	1:D:114:LEU:HD21	2.39	0.53
1:E:53:ASN:HD22	1:E:58:ASP:HB2	1.73	0.53
1:E:60:GLU:O	1:E:75:ILE:HA	2.09	0.53
1:B:57:ARG:HB2	1:B:60:GLU:HG2	1.91	0.52
1:C:53:ASN:HD21	1:C:137:GLN:HG3	1.67	0.52
1:D:192:ILE:CG2	1:D:196:VAL:HG13	2.30	0.52
1:D:135:GLN:HB3	1:D:144:PHE:CD1	2.45	0.52
2:F:45:LEU:O	2:F:47:PRO:CD	2.55	0.52
2:F:119:THR:HG22	2:F:129:PHE:HD1	1.74	0.52
1:E:13:ARG:HD2	1:E:13:ARG:C	2.35	0.52
1:D:58:ASP:C	1:D:60:GLU:H	2.16	0.52
1:B:92:VAL:HG22	1:B:93:HIS:N	2.24	0.52
1:D:78:HIS:CE1	1:D:120:ARG:NH2	2.78	0.52
1:C:144:PHE:HD1	1:C:144:PHE:H	1.58	0.52
1:E:56:GLY:O	1:E:57:ARG:HB2	2.09	0.51
1:D:8:VAL:CG1	1:D:9:PHE:N	2.73	0.51
1:E:71:TYR:O	1:E:81:THR:HG23	2.09	0.51
1:D:75:ILE:HG23	1:D:75:ILE:O	2.09	0.51
1:E:7:LYS:HA	1:E:200:PRO:HA	1.90	0.51
2:F:31:SER:CB	2:F:32:PRO:CD	2.89	0.51
2:F:70:THR:HG22	2:F:71:GLY:N	2.26	0.51
1:A:16:VAL:O	1:A:144:PHE:HB2	2.10	0.51
1:D:70:GLU:HG2	1:D:81:THR:CG2	2.41	0.51
1:E:75:ILE:HG12	1:E:119:LEU:HD11	1.92	0.51
1:E:34:THR:HG23	1:E:163:VAL:HA	1.92	0.51
2:F:18:GLN:HB2	2:F:110:TRP:CZ3	2.46	0.51
1:A:138:ASP:HB2	1:A:142:GLY:O	2.11	0.51
2:F:59:ASN:C	2:F:59:ASN:ND2	2.56	0.51
1:C:81:THR:HG22	1:C:82:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HZ2	1:A:141:GLY:CA	2.23	0.51
1:D:23:ILE:HD12	1:D:189:ASN:C	2.36	0.51
1:E:22:LEU:HB2	1:E:131:ILE:HB	1.93	0.51
1:A:195:TYR:CE1	1:A:197:ILE:HD11	2.46	0.50
1:C:58:ASP:CG	1:C:59:ASN:H	2.19	0.50
1:A:75:ILE:HG12	1:A:119:LEU:HD21	1.93	0.50
1:A:137:GLN:CG	1:A:141:GLY:HA2	2.40	0.50
1:A:203:TRP:H	1:A:203:TRP:CD1	2.29	0.50
1:E:109:ILE:HD13	1:E:114:LEU:HD11	1.94	0.50
1:C:182:ILE:O	1:C:183:LEU:HD23	2.11	0.50
1:B:5:SER:OG	1:B:186:GLN:HG2	2.11	0.50
2:F:99:GLU:HG2	2:F:100:GLY:N	2.26	0.50
1:B:33:PHE:CD1	1:B:33:PHE:C	2.89	0.50
1:B:16:VAL:HG11	1:B:143:LYS:HB3	1.94	0.50
1:D:54:THR:CG2	1:D:55:GLN:N	2.70	0.49
1:E:52:TYR:CD1	1:E:52:TYR:C	2.90	0.49
2:F:31:SER:HB3	2:F:32:PRO:CD	2.39	0.49
1:B:97:SER:O	1:B:105:ALA:HA	2.11	0.49
2:F:6:VAL:HB	2:F:27:GLN:HB2	1.94	0.49
2:F:45:LEU:HD13	2:F:47:PRO:HA	1.93	0.49
1:A:35:LEU:CD1	1:A:157:LEU:HD11	2.41	0.49
1:B:137:GLN:HG3	1:B:138:ASP:N	2.26	0.49
1:C:55:GLN:HE21	1:C:128:GLN:CB	2.19	0.49
1:A:153:GLU:CD	1:A:203:TRP:HE1	2.21	0.49
1:D:159:MET:HB3	1:D:183:LEU:HB2	1.95	0.49
2:F:17:LEU:HD21	2:F:89:VAL:CG2	2.40	0.49
2:F:149:TYR:O	2:F:150:HIS:HB3	2.13	0.49
1:C:197:ILE:CG2	1:C:198:ILE:N	2.76	0.48
1:C:109:ILE:HD13	1:C:114:LEU:HD11	1.94	0.48
1:D:87:LYS:NZ	1:D:87:LYS:HB3	2.27	0.48
1:A:35:LEU:O	1:A:95:CYS:HA	2.14	0.48
1:A:158:TYR:CE2	1:A:184:ASP:OD1	2.66	0.48
1:C:164:LEU:HB3	1:C:168:ASN:HB2	1.95	0.48
1:A:134:GLY:HA2	1:A:150:PHE:HB3	1.96	0.48
1:C:53:ASN:OD1	1:C:130:LYS:HB3	2.12	0.48
1:A:93:HIS:HD2	6:A:210:HOH:O	1.95	0.48
1:E:75:ILE:CD1	1:E:119:LEU:HG	2.35	0.48
1:A:91:PRO:HB2	5:F:179:GOL:H12	1.95	0.48
1:C:52:TYR:O	1:C:52:TYR:HD1	1.97	0.48
1:A:24:THR:HG23	1:A:182:ILE:O	2.14	0.48
1:A:29:PRO:HD3	1:A:127:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:THR:HG23	1:E:162:SER:O	2.13	0.48
1:A:37:PHE:HA	1:A:156:ASP:O	2.12	0.47
1:E:32:ASN:O	1:E:33:PHE:HB3	2.13	0.47
1:B:38:ARG:HD2	1:B:156:ASP:OD2	2.15	0.47
1:D:8:VAL:HG12	1:D:9:PHE:N	2.29	0.47
1:A:53:ASN:ND2	1:A:59:ASN:H	2.10	0.47
1:B:10:VAL:HG13	1:B:197:ILE:HB	1.97	0.47
1:C:180:ALA:HB3	1:C:184:ASP:HB2	1.96	0.47
1:D:138:ASP:HB2	1:D:143:LYS:HG2	1.96	0.47
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.78	0.47
1:D:75:ILE:HD13	1:D:75:ILE:C	2.40	0.47
1:A:8:VAL:HG21	1:A:153:GLU:OE1	2.15	0.47
1:C:195:TYR:HE1	1:C:197:ILE:HD11	1.81	0.47
1:A:130:LYS:HZ2	1:A:141:GLY:HA3	1.81	0.46
1:C:8:VAL:HG13	1:C:201:LEU:HB2	1.97	0.46
1:C:190:TYR:CD1	1:C:190:TYR:N	2.82	0.46
1:D:158:TYR:CZ	1:D:177:PRO:HG3	2.51	0.46
2:F:90:LEU:HD12	2:F:150:HIS:CA	2.45	0.46
1:C:32:ASN:HB3	1:C:99:GLU:HA	1.97	0.46
1:D:66:GLU:HG3	1:D:67:ARG:HG3	1.98	0.46
1:A:175:GLY:O	1:A:177:PRO:HD3	2.16	0.46
1:E:51:SER:HB3	1:E:137:GLN:HB2	1.98	0.46
1:E:75:ILE:O	1:E:75:ILE:HG13	2.15	0.46
1:C:53:ASN:ND2	1:C:137:GLN:CG	2.66	0.46
1:C:70:GLU:OE1	1:C:81:THR:HG21	2.16	0.46
1:C:174:GLN:HA	1:C:174:GLN:HE21	1.79	0.46
1:E:52:TYR:CB	1:E:61:LEU:HB2	2.33	0.46
1:E:201:LEU:HD21	1:E:204:VAL:OXT	2.16	0.46
2:F:131:ARG:H	2:F:131:ARG:HG2	1.51	0.46
1:C:158:TYR:CZ	1:C:177:PRO:HG3	2.51	0.46
1:E:87:LYS:HB3	1:E:87:LYS:HE2	1.53	0.46
1:C:75:ILE:HG23	1:C:75:ILE:O	2.16	0.46
1:D:36:CYS:O	1:D:37:PHE:HB3	2.15	0.46
1:D:23:ILE:HD12	1:D:189:ASN:O	2.16	0.46
1:E:22:LEU:N	1:E:22:LEU:HD12	2.31	0.46
1:E:53:ASN:HB2	1:E:58:ASP:HA	1.98	0.46
2:F:116:VAL:O	2:F:154:ASN:HB2	2.15	0.45
1:A:38:ARG:HB3	1:A:203:TRP:HZ3	1.81	0.45
1:A:203:TRP:CD1	1:A:203:TRP:N	2.82	0.45
1:A:29:PRO:N	1:A:127:ALA:HB2	2.31	0.45
1:B:16:VAL:CG1	1:B:143:LYS:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:PHE:O	1:E:97:SER:HA	2.17	0.45
1:B:35:LEU:O	1:B:95:CYS:HA	2.16	0.45
1:E:34:THR:HG22	1:E:97:SER:CB	2.46	0.45
2:F:5:ALA:O	2:F:76:SER:HB2	2.16	0.45
1:E:34:THR:CG2	1:E:163:VAL:HA	2.46	0.45
2:F:119:THR:CG2	2:F:129:PHE:CD1	2.95	0.45
1:A:197:ILE:N	1:A:197:ILE:CD1	2.80	0.45
1:E:135:GLN:HE21	1:E:135:GLN:CA	2.29	0.45
1:C:55:GLN:NE2	1:C:128:GLN:HB2	2.22	0.45
1:B:24:THR:CG2	1:B:25:PRO:HD2	2.47	0.45
1:B:176:THR:HG22	1:B:176:THR:O	2.17	0.45
1:B:204:VAL:HG23	1:B:204:VAL:OXT	2.17	0.45
1:B:52:TYR:CB	1:B:61:LEU:HB2	2.45	0.45
1:C:78:HIS:HD2	1:C:120:ARG:NE	2.15	0.45
1:E:104:ILE:O	1:E:104:ILE:HG13	2.17	0.45
2:F:122:GLN:HG3	2:F:149:TYR:CZ	2.52	0.45
1:E:35:LEU:HD12	1:E:158:TYR:O	2.16	0.44
2:F:103:ILE:O	2:F:103:ILE:HG12	2.17	0.44
1:D:87:LYS:HB3	1:D:87:LYS:HZ3	1.81	0.44
2:F:3:PRO:O	2:F:73:THR:HG22	2.17	0.44
1:C:103:GLY:O	1:C:118:GLY:HA2	2.18	0.44
1:D:128:GLN:N	1:D:129:PRO:HD3	2.31	0.44
1:D:135:GLN:NE2	1:D:144:PHE:HB3	2.32	0.44
1:B:75:ILE:HG13	1:B:119:LEU:CD2	2.44	0.44
1:C:22:LEU:N	1:C:22:LEU:HD12	2.33	0.44
1:C:195:TYR:CE1	1:C:197:ILE:HD11	2.52	0.44
2:F:92:THR:HB	2:F:94:HIS:O	2.17	0.44
1:B:69:GLY:O	1:B:83:LYS:HA	2.18	0.44
1:C:8:VAL:CG1	1:C:201:LEU:HD13	2.47	0.44
1:E:53:ASN:N	1:E:53:ASN:OD1	2.51	0.44
1:D:21:ASN:O	1:D:190:TYR:HA	2.17	0.44
2:F:89:VAL:HA	2:F:162:SER:OG	2.18	0.44
1:C:55:GLN:HE21	1:C:128:GLN:H	1.65	0.44
1:D:8:VAL:HG22	1:D:155:GLY:HA3	1.99	0.44
1:D:69:GLY:O	1:D:83:LYS:HA	2.18	0.44
1:D:199:LYS:HD3	1:D:200:PRO:HD3	1.99	0.44
1:E:72:SER:HB3	1:E:81:THR:OG1	2.18	0.44
1:E:74:TYR:CE2	1:E:79:LYS:HB3	2.53	0.44
1:E:103:GLY:O	1:E:119:LEU:N	2.49	0.44
2:F:142:ASN:HB2	2:F:144:SER:OG	2.17	0.44
1:A:24:THR:CG2	1:A:182:ILE:HG23	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:CD1	1:A:33:PHE:C	2.96	0.43
1:E:167:GLU:HG3	1:E:168:ASN:N	2.31	0.43
1:B:91:PRO:HB3	1:B:203:TRP:CE3	2.53	0.43
1:B:190:TYR:CD1	1:B:190:TYR:N	2.86	0.43
1:D:140:TYR:O	1:D:140:TYR:CD2	2.71	0.43
1:E:175:GLY:O	1:E:176:THR:HG23	2.18	0.43
1:E:197:ILE:HG22	1:E:198:ILE:N	2.33	0.43
1:E:12:PRO:HG2	1:E:195:TYR:CD2	2.54	0.43
1:E:33:PHE:C	1:E:33:PHE:CD1	2.95	0.43
2:F:70:THR:CG2	2:F:71:GLY:N	2.82	0.43
1:A:201:LEU:C	1:A:201:LEU:HD12	2.43	0.43
1:D:75:ILE:HG22	1:D:119:LEU:CD1	2.46	0.43
1:A:137:GLN:NE2	1:A:141:GLY:HA2	2.27	0.43
1:B:10:VAL:HG12	1:B:197:ILE:O	2.18	0.43
1:C:125:VAL:O	1:C:126:GLU:C	2.62	0.43
1:D:27:GLU:O	1:D:127:ALA:HB1	2.18	0.43
1:D:35:LEU:O	1:D:95:CYS:HA	2.19	0.43
1:D:37:PHE:HA	1:D:156:ASP:O	2.18	0.43
1:B:14:GLU:HG3	1:B:45:ARG:HH21	1.84	0.43
1:A:51:SER:HB2	1:A:132:VAL:HG22	2.01	0.43
1:C:14:GLU:HB3	1:C:151:VAL:HG21	2.01	0.43
1:C:59:ASN:O	1:C:60:GLU:C	2.61	0.43
1:D:58:ASP:OD2	1:D:138:ASP:HA	2.19	0.43
1:D:112:THR:HA	1:D:113:PRO:HD3	1.84	0.43
1:D:199:LYS:HD3	1:D:200:PRO:CD	2.49	0.43
1:E:135:GLN:HA	1:E:135:GLN:NE2	2.34	0.42
1:E:178:LEU:O	1:E:179:PRO:C	2.62	0.42
1:B:54:THR:HB	1:B:60:GLU:HG3	2.00	0.42
1:D:30:LEU:HB2	1:D:125:VAL:HB	2.01	0.42
1:E:54:THR:OG1	1:E:126:GLU:HB2	2.18	0.42
1:B:159:MET:O	1:B:182:ILE:HB	2.19	0.42
1:A:24:THR:HG22	1:A:25:PRO:HD2	2.01	0.42
1:A:54:THR:HG22	1:A:128:GLN:C	2.44	0.42
1:A:202:VAL:O	1:A:203:TRP:C	2.61	0.42
1:A:165:PRO:CD	1:A:168:ASN:HD22	2.22	0.42
1:D:16:VAL:O	1:D:144:PHE:HB2	2.20	0.42
1:D:34:THR:OG1	1:D:163:VAL:HA	2.19	0.42
1:D:81:THR:HG22	1:D:82:SER:N	2.34	0.42
1:E:61:LEU:HD23	1:E:75:ILE:HG22	2.00	0.42
1:E:84:VAL:HG22	1:E:114:LEU:CD1	2.49	0.42
2:F:105:LEU:N	2:F:105:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:HIS:HD2	1:B:1:HIS:O	2.02	0.42
1:A:106:GLU:CD	1:A:108:TRP:HE1	2.28	0.42
1:D:10:VAL:O	1:D:10:VAL:CG2	2.66	0.42
1:C:54:THR:HG22	1:C:57:ARG:HB2	2.00	0.42
1:C:75:ILE:HG22	1:C:119:LEU:CD1	2.46	0.42
1:C:197:ILE:HG22	1:C:198:ILE:N	2.34	0.42
1:C:204:VAL:HG11	2:F:155:ILE:O	2.19	0.42
1:C:58:ASP:CG	1:C:59:ASN:N	2.78	0.42
1:D:10:VAL:O	1:D:12:PRO:HD3	2.19	0.42
1:B:10:VAL:CG1	1:B:197:ILE:O	2.68	0.42
1:D:8:VAL:O	1:D:198:ILE:HA	2.20	0.42
1:B:36:CYS:HA	1:B:94:ILE:O	2.20	0.41
1:B:165:PRO:O	1:B:166:PRO:C	2.62	0.41
1:D:108:TRP:HA	1:D:112:THR:O	2.19	0.41
1:E:44:SER:HB3	3:E:207:SO4:O1	2.20	0.41
2:F:98:GLN:O	2:F:99:GLU:O	2.38	0.41
1:A:97:SER:O	1:A:105:ALA:HA	2.21	0.41
2:F:102:THR:HA	2:F:138:ILE:O	2.21	0.41
1:A:178:LEU:HG	1:A:179:PRO:HD2	2.02	0.41
1:C:97:SER:O	1:C:105:ALA:HA	2.20	0.41
1:E:60:GLU:CD	1:E:126:GLU:HG2	2.44	0.41
1:D:58:ASP:C	1:D:60:GLU:N	2.77	0.41
1:D:178:LEU:O	1:D:179:PRO:C	2.63	0.41
1:E:15:SER:OG	1:E:18:ASP:HB2	2.21	0.41
1:A:157:LEU:C	1:A:157:LEU:CD1	2.94	0.41
1:B:92:VAL:CG2	1:B:93:HIS:N	2.84	0.41
1:D:62:LEU:HB3	1:D:74:TYR:HB2	2.02	0.41
2:F:122:GLN:OE1	2:F:127:GLN:NE2	2.53	0.41
2:F:47:PRO:HG2	2:F:48:THR:HG22	2.02	0.41
1:B:81:THR:HG22	1:B:82:SER:N	2.35	0.41
1:C:174:GLN:NE2	1:C:174:GLN:CA	2.81	0.41
1:E:54:THR:HG22	1:E:55:GLN:OE1	2.20	0.41
1:B:54:THR:HG22	1:B:57:ARG:H	1.86	0.41
1:B:158:TYR:HA	1:B:183:LEU:O	2.21	0.41
1:B:201:LEU:HD21	1:B:203:TRP:CD2	2.56	0.41
1:C:24:THR:HG22	1:C:26:LEU:H	1.86	0.41
1:D:42:ASP:OD2	1:D:42:ASP:C	2.64	0.41
1:E:60:GLU:HG2	1:E:125:VAL:HG13	2.03	0.41
1:B:26:LEU:HD21	1:B:30:LEU:HD13	2.02	0.41
1:B:159:MET:HG2	1:B:182:ILE:HD12	2.02	0.41
1:C:52:TYR:O	1:C:52:TYR:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:PRO:CG	1:E:168:ASN:ND2	2.84	0.41
1:A:178:LEU:CD1	1:A:179:PRO:HD2	2.51	0.40
1:A:178:LEU:HD12	1:A:179:PRO:HD2	2.02	0.40
1:E:204:VAL:OXT	1:E:204:VAL:HG12	2.21	0.40
1:C:16:VAL:O	1:C:144:PHE:HD2	2.03	0.40
1:C:120:ARG:O	1:C:123:TYR:HB3	2.21	0.40
1:A:197:ILE:HG12	1:B:102:SER:HB2	2.01	0.40
1:C:136:GLU:OE1	1:C:148:GLN:OE1	2.40	0.40
1:D:46:ALA:HB2	1:D:66:GLU:O	2.21	0.40
1:D:101:SER:OG	1:D:102:SER:N	2.54	0.40
2:F:90:LEU:HD12	2:F:150:HIS:N	2.36	0.40
1:B:71:TYR:OH	1:B:86:GLU:OE1	2.33	0.40
1:C:57:ARG:HG2	1:C:57:ARG:H	1.38	0.40
1:D:11:PHE:CD2	1:D:11:PHE:N	2.90	0.40
1:D:165:PRO:HD2	1:D:168:ASN:ND2	2.33	0.40
1:E:10:VAL:O	1:E:12:PRO:CD	2.69	0.40
1:E:34:THR:HG22	1:E:97:SER:HB3	2.02	0.40
1:E:36:CYS:O	1:E:37:PHE:HB3	2.22	0.40
2:F:34:SER:HB2	5:F:179:GOL:C3	2.51	0.40
1:A:60:GLU:HG3	1:A:125:VAL:HG13	2.04	0.40
1:B:96:VAL:HA	1:B:106:GLU:O	2.22	0.40
1:C:158:TYR:CE1	1:C:177:PRO:HG3	2.56	0.40
1:E:52:TYR:CZ	1:E:129:PRO:HB3	2.56	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	202/204 (99%)	178 (88%)	22 (11%)	2 (1%)	12	38
1	B	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	202/204 (99%)	172 (85%)	24 (12%)	6 (3%)	3	12
1	D	202/204 (99%)	179 (89%)	17 (8%)	6 (3%)	3	12
1	E	202/204 (99%)	172 (85%)	24 (12%)	6 (3%)	3	12
2	F	169/177 (96%)	142 (84%)	23 (14%)	4 (2%)	4	17
All	All	1179/1197 (98%)	1030 (87%)	124 (10%)	25 (2%)	5	20

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	PHE
1	D	140	TYR
1	D	143	LYS
1	E	68	VAL
2	F	31	SER
2	F	99	GLU
1	B	127	ALA
1	C	181	ASN
1	D	56	GLY
1	E	29	PRO
1	E	59	ASN
1	C	180	ALA
1	E	18	ASP
1	E	179	PRO
1	E	187	ALA
1	C	126	GLU
1	C	139	SER
1	D	141	GLY
1	D	177	PRO
2	F	139	PRO
1	A	29	PRO
1	A	141	GLY
1	D	179	PRO
2	F	46	ILE
1	C	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/181 (99%)	159 (89%)	20 (11%)	6	19
1	B	180/181 (99%)	163 (91%)	17 (9%)	8	27
1	C	177/181 (98%)	159 (90%)	18 (10%)	7	23
1	D	176/181 (97%)	157 (89%)	19 (11%)	6	21
1	E	178/181 (98%)	158 (89%)	20 (11%)	6	19
2	F	146/163 (90%)	118 (81%)	28 (19%)	1	5
All	All	1036/1068 (97%)	914 (88%)	122 (12%)	5	17

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	24	THR
1	A	43	LEU
1	A	44	SER
1	A	53	ASN
1	A	54	THR
1	A	66	GLU
1	A	80	VAL
1	A	101	SER
1	A	130	LYS
1	A	132	VAL
1	A	138	ASP
1	A	139	SER
1	A	143	LYS
1	A	157	LEU
1	A	183	LEU
1	A	193	ARG
1	A	196	VAL
1	A	201	LEU
1	A	204	VAL
1	B	1	HIS
1	B	10	VAL
1	B	16	VAL
1	B	30	LEU
1	B	44	SER
1	B	54	THR
1	B	57	ARG

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Mol	Chain	Res	Type
1	B	66	GLU
1	B	73	LEU
1	B	80	VAL
1	B	129	PRO
1	B	146	ARG
1	B	166	PRO
1	B	170	LEU
1	B	183	LEU
1	B	196	VAL
1	B	201	LEU
1	C	2	THR
1	C	10	VAL
1	C	24	THR
1	C	26	LEU
1	C	27	GLU
1	C	43	LEU
1	C	53	ASN
1	C	55	GLN
1	C	57	ARG
1	C	65	LYS
1	C	101	SER
1	C	109	ILE
1	C	129	PRO
1	C	133	LEU
1	C	135	GLN
1	C	189	ASN
1	C	196	VAL
1	C	204	VAL
1	D	10	VAL
1	D	16	VAL
1	D	22	LEU
1	D	23	ILE
1	D	30	LEU
1	D	33	PHE
1	D	43	LEU
1	D	73	LEU
1	D	75	ILE
1	D	80	VAL
1	D	84	VAL
1	D	85	ILE
1	D	87	LYS
1	D	123	TYR

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Mol	Chain	Res	Type
1	D	135	GLN
1	D	170	LEU
1	D	183	LEU
1	D	196	VAL
1	D	203	TRP
1	E	10	VAL
1	E	30	LEU
1	E	43	LEU
1	E	52	TYR
1	E	54	THR
1	E	68	VAL
1	E	79	LYS
1	E	80	VAL
1	E	83	LYS
1	E	84	VAL
1	E	96	VAL
1	E	101	SER
1	E	106	GLU
1	E	131	ILE
1	E	133	LEU
1	E	157	LEU
1	E	179	PRO
1	E	196	VAL
1	E	202	VAL
1	E	203	TRP
2	F	9	LEU
2	F	10	GLU
2	F	15	ASN
2	F	25	THR
2	F	30	ARG
2	F	31	SER
2	F	33	GLU
2	F	34	SER
2	F	45	LEU
2	F	48	THR
2	F	51	GLN
2	F	59	ASN
2	F	73	THR
2	F	81	LEU
2	F	82	THR
2	F	89	VAL
2	F	92	THR

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Mol	Chain	Res	Type
2	F	103	ILE
2	F	104	MET
2	F	110	TRP
2	F	116	VAL
2	F	126	SER
2	F	131	ARG
2	F	132	LEU
2	F	151	CYS
2	F	158	THR
2	F	165	VAL
2	F	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	31	GLN
1	A	59	ASN
1	A	93	HIS
1	A	135	GLN
1	A	137	GLN
1	A	148	GLN
1	A	168	ASN
1	B	1	HIS
1	B	78	HIS
1	B	93	HIS
1	B	121	GLN
1	B	128	GLN
1	B	135	GLN
1	B	148	GLN
1	B	168	ASN
1	B	174	GLN
1	B	189	ASN
1	C	31	GLN
1	C	55	GLN
1	C	59	ASN
1	C	78	HIS
1	C	135	GLN
1	C	137	GLN
1	C	174	GLN
1	D	1	HIS
1	D	59	ASN

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Mol	Chain	Res	Type
1	D	135	GLN
1	D	168	ASN
1	D	189	ASN
1	E	135	GLN
1	E	148	GLN
1	E	168	ASN
2	F	38	GLN
2	F	59	ASN
2	F	60	ASN
2	F	69	GLN
2	F	72	GLN
2	F	80	HIS
2	F	123	ASN
2	F	127	GLN
2	F	142	ASN
2	F	150	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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
3	SO4	E	205	-	4,4,4	0.41	0	6,6,6	0.12	0
3	SO4	E	207	-	4,4,4	0.35	0	6,6,6	0.07	0
5	GOL	F	179	-	5,5,5	0.28	0	5,5,5	0.32	0
4	NAG	B	208	1	14,14,15	0.63	0	17,19,21	0.67	0
4	NAG	E	208	1	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
3	SO4	B	206	-	4,4,4	0.32	0	6,6,6	0.26	0
3	SO4	C	207	-	4,4,4	0.38	0	6,6,6	0.07	0
4	NAG	C	208	1	14,14,15	0.60	0	17,19,21	0.64	0
3	SO4	E	206	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	A	205	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	F	178	-	4,4,4	0.35	0	6,6,6	0.18	0
4	NAG	D	208	1	14,14,15	0.72	0	17,19,21	0.60	0
3	SO4	A	207	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	C	206	-	4,4,4	0.39	0	6,6,6	0.18	0
3	SO4	C	205	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	B	205	-	4,4,4	0.32	0	6,6,6	0.15	0
3	SO4	D	205	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	D	206	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	B	207	-	4,4,4	0.35	0	6,6,6	0.13	0
3	SO4	D	207	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	A	206	-	4,4,4	0.39	0	6,6,6	0.14	0
4	NAG	A	208	1	14,14,15	0.55	0	17,19,21	0.85	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
4	NAG	C	208	1	-	3/6/23/26	0/1/1/1
5	GOL	F	179	-	-	0/4/4/4	-
4	NAG	B	208	1	-	4/6/23/26	0/1/1/1
4	NAG	E	208	1	-	2/6/23/26	0/1/1/1
4	NAG	D	208	1	-	3/6/23/26	0/1/1/1
4	NAG	A	208	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	208	NAG	C1-C2	2.02	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	208	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	208	NAG	C3-C2-N2-C7
4	A	208	NAG	C8-C7-N2-C2
4	A	208	NAG	O7-C7-N2-C2
4	B	208	NAG	C3-C2-N2-C7
4	C	208	NAG	C8-C7-N2-C2
4	C	208	NAG	O7-C7-N2-C2
4	E	208	NAG	C8-C7-N2-C2
4	E	208	NAG	O7-C7-N2-C2
4	B	208	NAG	C8-C7-N2-C2
4	B	208	NAG	O7-C7-N2-C2
4	C	208	NAG	C3-C2-N2-C7
4	B	208	NAG	O5-C5-C6-O6
4	D	208	NAG	C1-C2-N2-C7
4	D	208	NAG	C3-C2-N2-C7
4	D	208	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	207	SO4	1	0
5	F	179	GOL	3	0
4	A	208	NAG	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 ⓘ

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, 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	204/204 (100%)	-0.12	9 (4%) 39 31	19, 36, 69, 111	0
1	B	204/204 (100%)	-0.40	1 (0%) 87 82	20, 34, 57, 77	0
1	C	204/204 (100%)	0.21	9 (4%) 39 31	24, 47, 93, 119	0
1	D	204/204 (100%)	0.20	11 (5%) 31 24	31, 51, 95, 120	0
1	E	204/204 (100%)	0.36	7 (3%) 48 39	27, 58, 93, 117	0
2	F	171/177 (96%)	0.72	25 (14%) 6 4	20, 68, 92, 109	0
All	All	1191/1197 (99%)	0.15	62 (5%) 33 25	19, 48, 91, 120	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	TYR	4.8
1	D	145	ASP	4.7
2	F	171	VAL	4.7
1	D	143	LYS	4.4
1	D	142	GLY	4.3
1	E	27	GLU	4.0
1	C	139	SER	4.0
1	D	144	PHE	3.7
1	C	141	GLY	3.6
1	C	145	ASP	3.6
1	E	145	ASP	3.5
2	F	107	CYS	3.5
2	F	98	GLN	3.4
2	F	169	VAL	3.4
1	E	140	TYR	3.2
1	D	141	GLY	3.2
2	F	100	GLY	3.1
1	C	57	ARG	3.1
1	D	140	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	204	VAL	3.0
2	F	121	PHE	3.0
1	D	139	SER	2.9
2	F	127	GLN	2.8
2	F	157	TYR	2.8
1	E	204	VAL	2.8
1	A	145	ASP	2.8
1	A	56	GLY	2.8
1	A	141	GLY	2.7
1	D	58	ASP	2.7
1	A	204	VAL	2.7
2	F	118	VAL	2.7
2	F	143	HIS	2.6
2	F	31	SER	2.6
1	C	127	ALA	2.6
1	D	27	GLU	2.5
2	F	167	ILE	2.4
2	F	34	SER	2.4
1	C	18	ASP	2.4
2	F	1	ALA	2.4
1	C	138	ASP	2.4
2	F	139	PRO	2.4
2	F	104	MET	2.3
1	A	139	SER	2.3
1	E	128	GLN	2.3
2	F	165	VAL	2.3
2	F	91	GLN	2.2
1	A	140	TYR	2.2
1	E	56	GLY	2.2
1	D	16	VAL	2.2
2	F	119	THR	2.2
1	A	58	ASP	2.2
1	A	143	LYS	2.2
2	F	115	LEU	2.2
1	B	127	ALA	2.2
1	C	143	LYS	2.1
1	E	141	GLY	2.1
1	A	153	GLU	2.1
2	F	33	GLU	2.1
2	F	145	HIS	2.0
2	F	120	PHE	2.0
2	F	141	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	152	THR	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 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	D	208	14/15	0.53	0.16	56,74,84,91	0
4	NAG	E	208	14/15	0.59	0.13	67,78,87,91	0
4	NAG	A	208	14/15	0.63	0.15	53,67,80,82	0
4	NAG	C	208	14/15	0.66	0.15	64,76,85,86	0
4	NAG	B	208	14/15	0.78	0.14	48,64,79,92	0
3	SO4	C	206	5/5	0.79	0.11	77,82,86,93	0
3	SO4	E	206	5/5	0.81	0.11	85,85,89,91	0
3	SO4	D	205	5/5	0.82	0.12	82,82,94,96	0
5	GOL	F	179	6/6	0.82	0.18	48,63,66,69	0
3	SO4	C	207	5/5	0.84	0.17	72,80,85,85	0
3	SO4	B	205	5/5	0.85	0.16	81,83,87,94	0
3	SO4	A	206	5/5	0.86	0.09	66,67,74,74	0
3	SO4	A	205	5/5	0.88	0.10	69,69,79,89	0
3	SO4	D	206	5/5	0.89	0.10	67,76,84,85	0
3	SO4	F	178	5/5	0.89	0.10	73,76,80,87	0
3	SO4	E	205	5/5	0.91	0.09	73,75,92,95	0
3	SO4	B	207	5/5	0.92	0.07	67,68,72,72	0
3	SO4	C	205	5/5	0.92	0.10	62,71,75,83	0
3	SO4	A	207	5/5	0.92	0.12	61,63,71,74	0
3	SO4	E	207	5/5	0.93	0.12	75,75,79,80	0
3	SO4	D	207	5/5	0.93	0.08	76,77,86,88	0
3	SO4	B	206	5/5	0.96	0.09	48,57,63,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.