



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:48 AM GMT

PDB ID : 1KBV
Title : NITRITE-SOAKED CRYSTAL STRUCTURE OF THE SOLUBLE DOMAIN OF ANIA FROM NEISSERIA GONORRHOEAE
Authors : Boulanger, M.J.; Murphy, M.E.P.
Deposited on : 2001-11-06
Resolution : 1.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

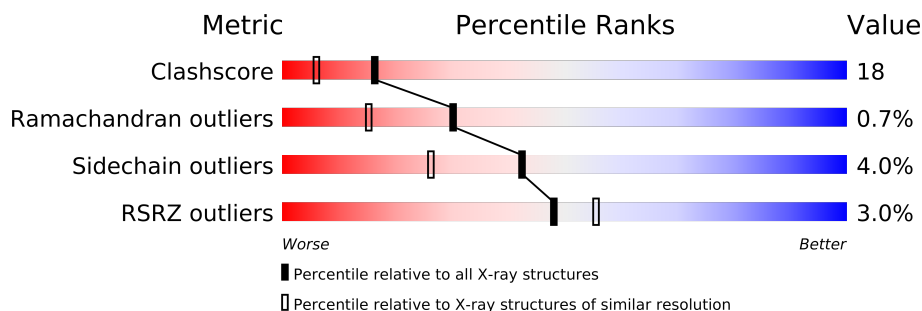
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	
1	E	327	
1	F	327	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NO2	A	2504	-	X
3	NO2	C	2505	-	X
3	NO2	E	2507	-	X
3	NO2	F	2508	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15834 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Major outer membrane protein PAN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	B	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	C	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	D	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	E	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			
1	F	302	Total	C	N	O	S	0	0	0
			2291	1461	385	435	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP Q02219
A	209	ALA	SER	SEE REMARK 999	UNP Q02219
A	210	LEU	ILE	SEE REMARK 999	UNP Q02219
A	211	THR	ALA	SEE REMARK 999	UNP Q02219
A	283	ASN	SER	SEE REMARK 999	UNP Q02219
A	325	VAL	-	CLONING ARTIFACT	UNP Q02219
A	326	PRO	-	CLONING ARTIFACT	UNP Q02219
A	327	ARG	-	CLONING ARTIFACT	UNP Q02219
B	1	MET	-	INITIATING MET	UNP Q02219
B	209	ALA	SER	SEE REMARK 999	UNP Q02219
B	210	LEU	ILE	SEE REMARK 999	UNP Q02219
B	211	THR	ALA	SEE REMARK 999	UNP Q02219
B	283	ASN	SER	SEE REMARK 999	UNP Q02219
B	325	VAL	-	CLONING ARTIFACT	UNP Q02219
B	326	PRO	-	CLONING ARTIFACT	UNP Q02219
B	327	ARG	-	CLONING ARTIFACT	UNP Q02219
C	1	MET	-	INITIATING MET	UNP Q02219

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Chain	Residue	Modelled	Actual	Comment	Reference
C	209	ALA	SER	SEE REMARK 999	UNP Q02219
C	210	LEU	ILE	SEE REMARK 999	UNP Q02219
C	211	THR	ALA	SEE REMARK 999	UNP Q02219
C	283	ASN	SER	SEE REMARK 999	UNP Q02219
C	325	VAL	-	CLONING ARTIFACT	UNP Q02219
C	326	PRO	-	CLONING ARTIFACT	UNP Q02219
C	327	ARG	-	CLONING ARTIFACT	UNP Q02219
D	1	MET	-	INITIATING MET	UNP Q02219
D	209	ALA	SER	SEE REMARK 999	UNP Q02219
D	210	LEU	ILE	SEE REMARK 999	UNP Q02219
D	211	THR	ALA	SEE REMARK 999	UNP Q02219
D	283	ASN	SER	SEE REMARK 999	UNP Q02219
D	325	VAL	-	CLONING ARTIFACT	UNP Q02219
D	326	PRO	-	CLONING ARTIFACT	UNP Q02219
D	327	ARG	-	CLONING ARTIFACT	UNP Q02219
E	1	MET	-	INITIATING MET	UNP Q02219
E	209	ALA	SER	SEE REMARK 999	UNP Q02219
E	210	LEU	ILE	SEE REMARK 999	UNP Q02219
E	211	THR	ALA	SEE REMARK 999	UNP Q02219
E	283	ASN	SER	SEE REMARK 999	UNP Q02219
E	325	VAL	-	CLONING ARTIFACT	UNP Q02219
E	326	PRO	-	CLONING ARTIFACT	UNP Q02219
E	327	ARG	-	CLONING ARTIFACT	UNP Q02219
F	1	MET	-	INITIATING MET	UNP Q02219
F	209	ALA	SER	SEE REMARK 999	UNP Q02219
F	210	LEU	ILE	SEE REMARK 999	UNP Q02219
F	211	THR	ALA	SEE REMARK 999	UNP Q02219
F	283	ASN	SER	SEE REMARK 999	UNP Q02219
F	325	VAL	-	CLONING ARTIFACT	UNP Q02219
F	326	PRO	-	CLONING ARTIFACT	UNP Q02219
F	327	ARG	-	CLONING ARTIFACT	UNP Q02219

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

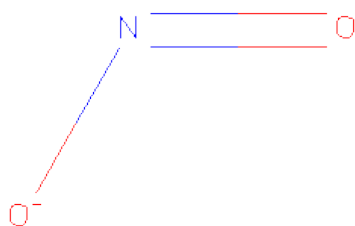
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is NITRITE ION (three-letter code: NO₂) (formula: NO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	C	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	E	1	Total	N	O	0	0
			3	1	2		
3	F	1	Total	N	O	0	0
			3	1	2		
3	D	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	377	Total	O	0	0
			377	377		

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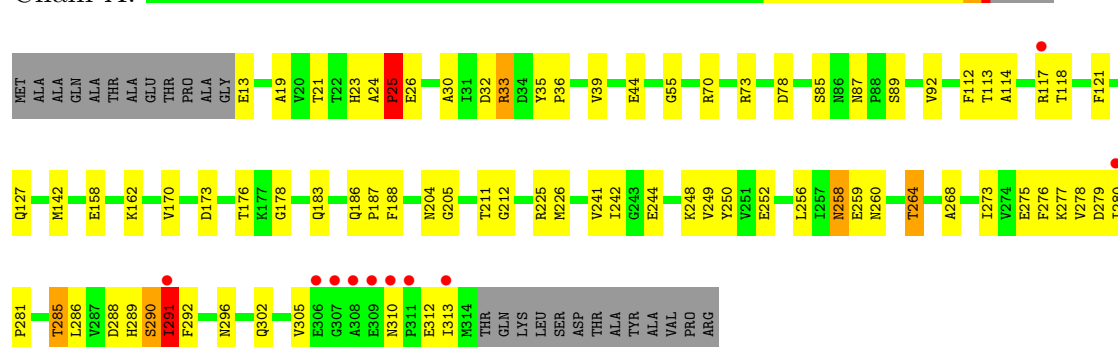
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	353	Total 353	O 353	0	0
4	C	310	Total 310	O 310	0	0
4	D	371	Total 371	O 371	0	0
4	E	317	Total 317	O 317	0	0
4	F	330	Total 330	O 330	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

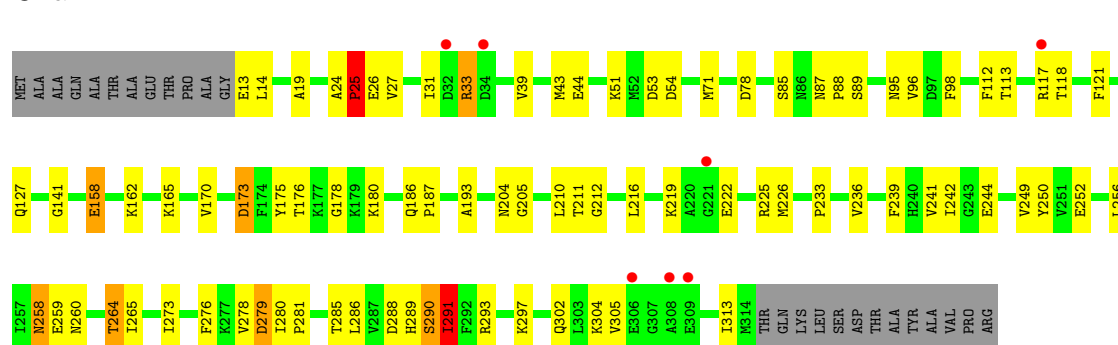
• Molecule 1: Major outer membrane protein PAN 1

Chain A:



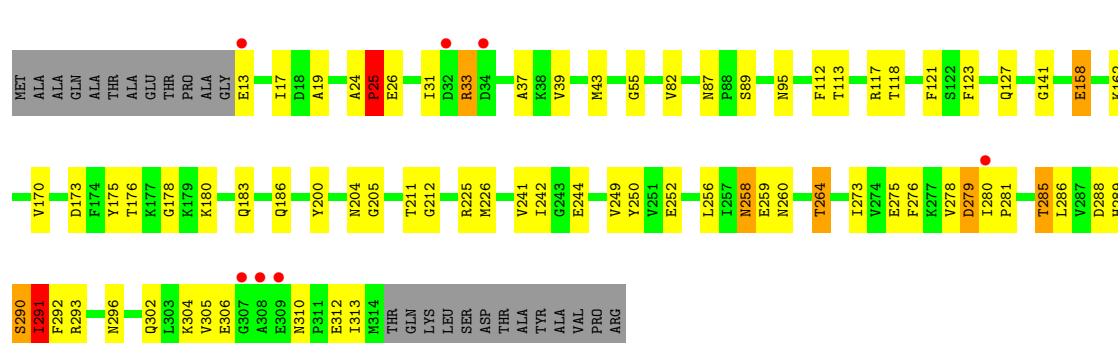
• Molecule 1: Major outer membrane protein PAN 1

Chain B:



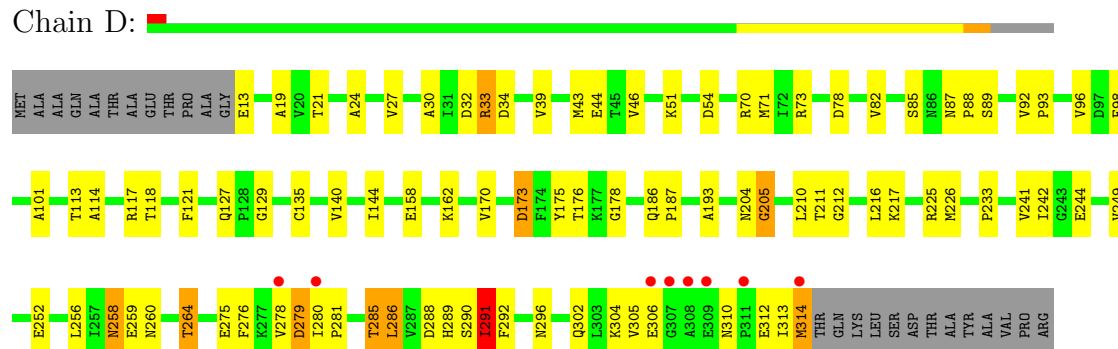
• Molecule 1: Major outer membrane protein PAN 1

Chain C:



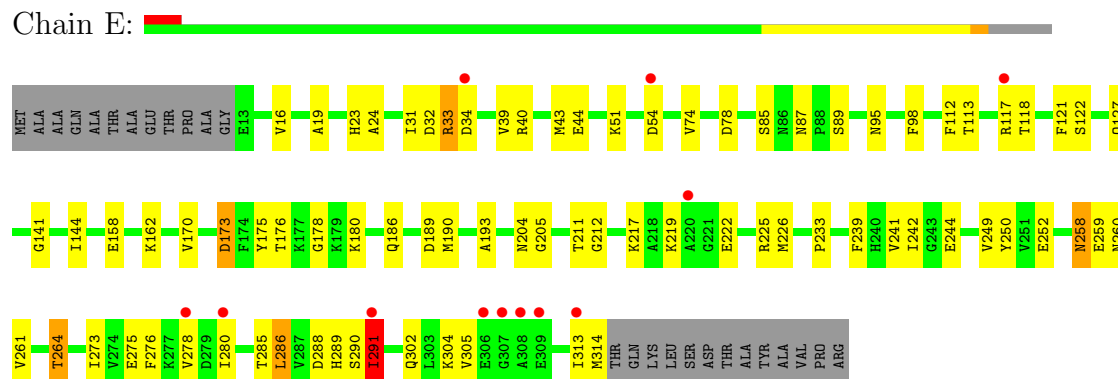
- Molecule 1: Major outer membrane protein PAN 1

Chain D:



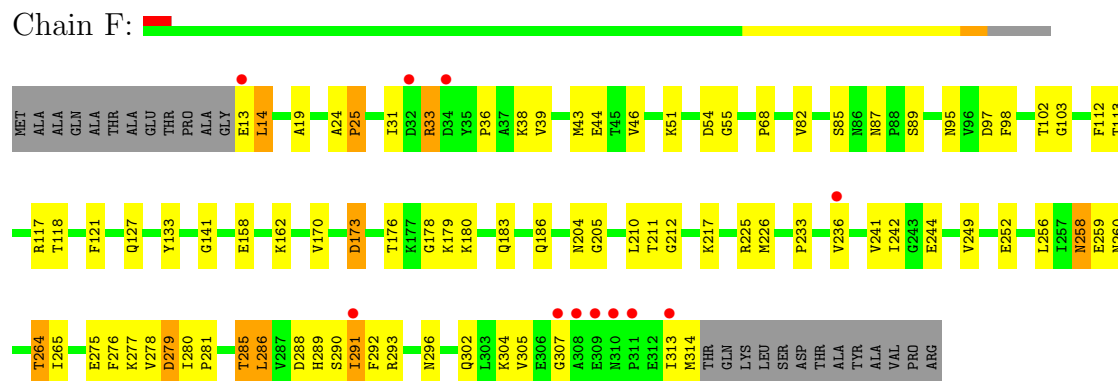
- Molecule 1: Major outer membrane protein PAN 1

Chain E:



- Molecule 1: Major outer membrane protein PAN 1

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.29Å 98.09Å 102.30Å 83.89° 74.14° 73.32°	Depositor
Resolution (Å)	49.18 – 1.95 49.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	87.2 (49.18-1.95) 85.7 (49.18-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.23 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.223 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.6	EDS
Estimated twinning fraction	0.075 for -h,-l,-k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 149119 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15834	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NO2, CU

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	0.41	0/2346	0.90	7/3185 (0.2%)
1	B	0.42	0/2346	0.90	6/3185 (0.2%)
1	C	0.41	0/2346	0.90	6/3185 (0.2%)
1	D	0.41	0/2346	0.86	5/3185 (0.2%)
1	E	0.40	0/2346	0.81	5/3185 (0.2%)
1	F	0.43	1/2346 (0.0%)	0.90	6/3185 (0.2%)
All	All	0.41	1/14076 (0.0%)	0.88	35/19110 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	293	ARG	C-O	5.42	1.33	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ALA	C-N-CD	-21.89	72.44	120.60
1	A	24	ALA	C-N-CD	-21.78	72.68	120.60
1	B	24	ALA	C-N-CD	-21.78	72.69	120.60
1	F	24	ALA	C-N-CD	-19.83	76.98	120.60
1	D	24	ALA	C-N-CD	-18.24	80.48	120.60
1	F	24	ALA	C-N-CA	13.75	179.74	122.00
1	A	24	ALA	C-N-CA	12.32	173.76	122.00
1	B	24	ALA	C-N-CA	12.27	173.51	122.00
1	D	24	ALA	C-N-CA	12.12	172.91	122.00
1	C	24	ALA	C-N-CA	12.08	172.74	122.00
1	E	24	ALA	C-N-CD	-12.06	94.07	120.60
1	E	24	ALA	C-N-CA	8.24	156.61	122.00
1	C	290	SER	N-CA-C	-7.54	90.64	111.00
1	A	290	SER	N-CA-C	-7.49	90.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	SER	N-CA-C	-7.48	90.80	111.00
1	D	290	SER	N-CA-C	-7.46	90.87	111.00
1	F	290	SER	N-CA-C	-7.43	90.94	111.00
1	B	290	SER	N-CA-C	-7.35	91.17	111.00
1	C	25	PRO	CA-N-CD	-7.01	101.68	111.50
1	A	25	PRO	CA-N-CD	-6.74	102.07	111.50
1	B	25	PRO	CA-N-CD	-6.65	102.19	111.50
1	F	205	GLY	N-CA-C	6.23	128.68	113.10
1	F	25	PRO	CA-N-CD	-6.23	102.78	111.50
1	E	205	GLY	N-CA-C	6.15	128.48	113.10
1	C	205	GLY	N-CA-C	6.11	128.38	113.10
1	A	288	ASP	N-CA-C	-6.07	94.60	111.00
1	B	205	GLY	N-CA-C	6.05	128.23	113.10
1	B	288	ASP	N-CA-C	-6.04	94.69	111.00
1	C	288	ASP	N-CA-C	-6.02	94.74	111.00
1	D	205	GLY	N-CA-C	5.91	127.87	113.10
1	E	288	ASP	N-CA-C	-5.89	95.10	111.00
1	A	205	GLY	N-CA-C	5.82	127.65	113.10
1	D	288	ASP	N-CA-C	-5.72	95.54	111.00
1	F	288	ASP	N-CA-C	-5.68	95.66	111.00
1	A	24	ALA	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2291	0	2234	94	0
1	B	2291	0	2234	82	0
1	C	2291	0	2234	77	0
1	D	2291	0	2234	107	0
1	E	2291	0	2234	87	0
1	F	2291	0	2234	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	0	2	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
3	E	3	0	0	1	0
3	F	3	0	0	1	0
4	A	377	0	0	12	0
4	B	353	0	0	4	0
4	C	310	0	0	5	0
4	D	371	0	0	16	0
4	E	317	0	0	10	0
4	F	330	0	0	8	0
All	All	15834	0	13404	493	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (493) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:278:VAL:HG11	1:E:305:VAL:HG21	1.22	1.18
1:C:278:VAL:HG11	1:C:305:VAL:HG21	1.31	1.10
1:B:278:VAL:HG11	1:B:305:VAL:HG21	1.34	1.09
1:D:278:VAL:HG11	1:D:305:VAL:HG21	1.40	1.03
1:E:249:VAL:HG11	1:E:264:THR:HG21	1.42	1.01
1:F:278:VAL:HG11	1:F:305:VAL:HG21	1.38	1.01
1:A:249:VAL:HG11	1:A:264:THR:HG21	1.50	0.94
1:A:278:VAL:HG11	1:A:305:VAL:HG21	1.50	0.94
1:B:249:VAL:HG11	1:B:264:THR:HG21	1.49	0.93
1:D:249:VAL:HG11	1:D:264:THR:HG21	1.52	0.92
1:B:51:LYS:HE3	4:B:675:HOH:O	1.71	0.90
1:E:144:ILE:HD13	1:F:291:ILE:CD1	2.03	0.88
1:A:117:ARG:HD3	4:A:2546:HOH:O	1.72	0.87
1:F:258:ASN:HD22	1:F:259:GLU:H	1.22	0.86
1:C:249:VAL:HG11	1:C:264:THR:HG21	1.56	0.86
1:F:176:THR:HG23	1:F:186:GLN:HB3	1.57	0.86
1:D:252:GLU:OE1	1:E:264:THR:HG22	1.76	0.85
1:E:144:ILE:CD1	1:F:291:ILE:HD13	2.08	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:280:ILE:HD11	1:F:313:ILE:HB	1.61	0.83
3:A:2504:NO2:N	1:B:242:ILE:HG12	1.93	0.82
1:D:32:ASP:CB	4:D:2790:HOH:O	2.28	0.81
1:A:113:THR:HA	1:A:117:ARG:NH1	1.96	0.81
1:A:252:GLU:OE1	1:B:264:THR:HG22	1.80	0.80
1:B:244:GLU:HG2	1:B:276:PHE:CD1	2.17	0.80
1:B:87:ASN:HD22	1:B:89:SER:H	1.28	0.80
1:E:280:ILE:HD11	1:E:313:ILE:HB	1.63	0.80
1:F:242:ILE:HG12	3:F:2508:NO2:N	1.97	0.80
1:D:176:THR:HG23	1:D:186:GLN:HB3	1.64	0.79
1:D:314:MET:HG3	1:F:103:GLY:HA3	1.63	0.79
1:E:113:THR:HG23	1:E:117:ARG:HD2	1.64	0.79
1:C:258:ASN:HD22	1:C:259:GLU:H	1.27	0.79
1:B:176:THR:HG23	1:B:186:GLN:HB3	1.63	0.79
1:D:117:ARG:HD3	4:D:2786:HOH:O	1.81	0.78
1:A:242:ILE:HD12	1:A:285:THR:HG23	1.65	0.78
1:A:176:THR:HG22	1:A:178:GLY:O	1.83	0.78
1:A:113:THR:HA	1:A:117:ARG:HH11	1.49	0.78
1:D:140:VAL:O	1:D:144:ILE:HD13	1.84	0.78
1:A:113:THR:HG23	1:A:117:ARG:HD2	1.66	0.78
1:A:225:ARG:HG3	1:A:275:GLU:HG2	1.66	0.76
1:D:280:ILE:HD11	1:D:313:ILE:HB	1.64	0.76
1:C:117:ARG:HG2	1:C:118:THR:N	2.00	0.76
1:F:225:ARG:HG3	1:F:275:GLU:HG2	1.69	0.75
1:E:242:ILE:HG12	3:E:2507:NO2:N	2.01	0.75
1:D:51:LYS:HE3	1:D:54:ASP:HA	1.69	0.75
1:C:278:VAL:HG11	1:C:305:VAL:CG2	2.13	0.75
1:A:242:ILE:HG12	3:A:2506:NO2:N	2.01	0.75
1:C:176:THR:HG23	1:C:186:GLN:HB3	1.69	0.75
1:A:87:ASN:HD22	1:A:89:SER:H	1.35	0.74
1:B:280:ILE:CD1	1:B:313:ILE:HB	2.17	0.74
1:D:70:ARG:CZ	4:D:2603:HOH:O	2.35	0.73
1:F:278:VAL:HG11	1:F:305:VAL:CG2	2.17	0.73
1:E:144:ILE:HD12	1:F:291:ILE:HD13	1.70	0.73
1:B:176:THR:HG22	1:B:178:GLY:O	1.89	0.73
1:E:176:THR:HG22	1:E:178:GLY:O	1.89	0.73
1:E:280:ILE:CD1	1:E:313:ILE:HB	2.18	0.73
1:D:258:ASN:HD22	1:D:259:GLU:H	1.37	0.72
1:A:117:ARG:HG2	1:A:118:THR:N	2.04	0.72
1:F:31:ILE:CG2	1:F:33:ARG:HG3	2.18	0.72
1:C:113:THR:HG23	1:C:117:ARG:HD2	1.72	0.72
1:D:176:THR:HG22	1:D:178:GLY:O	1.90	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:242:ILE:HG12	3:C:2505:NO2:N	2.04	0.72
1:A:32:ASP:CB	4:A:2599:HOH:O	2.38	0.71
1:D:225:ARG:HG3	1:D:275:GLU:HG2	1.73	0.71
1:A:264:THR:HG22	1:C:252:GLU:OE1	1.91	0.71
1:C:176:THR:HG22	1:C:178:GLY:O	1.90	0.71
1:D:127:GLN:HE21	1:E:260:ASN:HD22	1.37	0.71
1:E:117:ARG:HG2	1:E:118:THR:N	2.04	0.70
1:C:87:ASN:HD22	1:C:89:SER:H	1.37	0.70
1:B:280:ILE:HD11	1:B:313:ILE:HB	1.75	0.69
1:F:291:ILE:CD1	4:F:2526:HOH:O	2.41	0.69
1:F:117:ARG:HG2	1:F:118:THR:N	2.07	0.69
1:C:280:ILE:CD1	1:C:313:ILE:HB	2.23	0.69
1:B:117:ARG:HG2	1:B:118:THR:N	2.05	0.69
1:F:258:ASN:HD22	1:F:259:GLU:N	1.89	0.69
1:F:280:ILE:CD1	1:F:313:ILE:HB	2.22	0.69
1:E:162:LYS:HA	1:E:162:LYS:HE2	1.75	0.69
1:A:258:ASN:HD22	1:A:259:GLU:H	1.40	0.68
1:D:242:ILE:HG12	3:D:2509:NO2:N	2.07	0.68
1:A:127:GLN:HE21	1:B:260:ASN:HD22	1.41	0.68
1:F:176:THR:HG22	1:F:178:GLY:O	1.93	0.68
1:B:278:VAL:HG11	1:B:305:VAL:CG2	2.19	0.68
1:A:211:THR:HG22	1:A:212:GLY:N	2.09	0.68
1:B:280:ILE:HG13	1:B:313:ILE:HD12	1.76	0.68
1:D:13:GLU:N	4:D:2660:HOH:O	2.27	0.67
1:D:211:THR:HG22	1:D:212:GLY:N	2.08	0.67
1:B:162:LYS:HA	1:B:162:LYS:HE2	1.77	0.67
1:F:162:LYS:HA	1:F:162:LYS:HE2	1.76	0.67
1:E:144:ILE:HD13	1:F:291:ILE:HD11	1.75	0.67
1:F:13:GLU:N	4:F:2541:HOH:O	2.27	0.67
1:E:173:ASP:OD1	1:E:233:PRO:HD2	1.95	0.67
1:D:264:THR:HG22	1:F:252:GLU:OE1	1.94	0.66
1:B:113:THR:HG23	1:B:117:ARG:HD2	1.78	0.66
1:C:162:LYS:HE2	1:C:162:LYS:HA	1.77	0.66
1:E:19:ALA:HB2	1:E:39:VAL:CG1	2.26	0.66
1:D:278:VAL:HG11	1:D:305:VAL:CG2	2.21	0.66
1:E:176:THR:HG23	1:E:186:GLN:HB3	1.77	0.66
1:A:278:VAL:HG11	1:A:305:VAL:CG2	2.25	0.66
1:E:278:VAL:HG11	1:E:305:VAL:CG2	2.14	0.65
1:F:87:ASN:HD22	1:F:89:SER:H	1.44	0.65
1:B:117:ARG:HG2	1:B:118:THR:H	1.61	0.65
1:A:280:ILE:CD1	1:A:313:ILE:HB	2.26	0.65
1:B:19:ALA:HB2	1:B:39:VAL:CG1	2.25	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:280:ILE:CD1	1:D:313:ILE:HB	2.27	0.65
1:C:31:ILE:CG2	1:C:33:ARG:HG3	2.27	0.65
1:F:249:VAL:HG11	1:F:264:THR:HG21	1.79	0.64
1:A:176:THR:HG23	1:A:186:GLN:HB3	1.79	0.64
1:C:242:ILE:HB	1:C:285:THR:HG23	1.80	0.64
1:B:211:THR:HG22	1:B:212:GLY:N	2.11	0.64
1:C:117:ARG:HG2	1:C:118:THR:H	1.63	0.64
1:F:278:VAL:CG1	1:F:305:VAL:HG11	2.27	0.64
1:A:278:VAL:CG1	1:A:305:VAL:HG11	2.27	0.64
1:E:258:ASN:HD22	1:E:259:GLU:H	1.45	0.64
1:D:93:PRO:HD2	4:D:2852:HOH:O	1.96	0.64
1:C:55:GLY:HA3	1:C:183:GLN:HE22	1.62	0.64
1:E:117:ARG:HG2	1:E:118:THR:H	1.62	0.63
1:A:252:GLU:OE1	1:B:264:THR:CG2	2.47	0.63
1:A:242:ILE:HD12	1:A:285:THR:CG2	2.28	0.63
1:A:114:ALA:H	1:A:117:ARG:CZ	2.10	0.63
1:E:244:GLU:HG2	1:E:276:PHE:CD1	2.34	0.63
1:D:211:THR:HG23	1:D:302:GLN:CD	2.19	0.63
1:E:280:ILE:HG13	1:E:313:ILE:HD12	1.80	0.63
1:C:258:ASN:HD22	1:C:259:GLU:N	1.96	0.63
1:C:211:THR:HG22	1:C:212:GLY:N	2.14	0.63
1:A:256:LEU:HB2	1:B:258:ASN:ND2	2.14	0.63
1:D:170:VAL:H	1:D:204:ASN:ND2	1.97	0.62
1:E:225:ARG:HG3	1:E:275:GLU:HG2	1.81	0.62
1:E:289:HIS:C	1:E:291:ILE:N	2.53	0.62
1:E:252:GLU:OE1	1:F:264:THR:HG23	2.00	0.62
1:D:211:THR:CG2	1:D:212:GLY:N	2.63	0.62
1:D:217:LYS:HE2	1:D:304:LYS:HD3	1.82	0.62
1:D:87:ASN:HD22	1:D:89:SER:H	1.48	0.62
1:E:211:THR:HG22	1:E:212:GLY:N	2.14	0.62
1:F:13:GLU:O	1:F:13:GLU:HG3	1.99	0.62
1:F:19:ALA:HB2	1:F:39:VAL:HG12	1.81	0.61
1:A:226:MET:HE1	1:A:241:VAL:HG21	1.82	0.61
1:F:278:VAL:HG12	1:F:305:VAL:HG11	1.82	0.61
1:F:291:ILE:HD12	4:F:2526:HOH:O	2.01	0.61
1:B:51:LYS:HE2	1:B:53:ASP:O	2.01	0.61
1:F:242:ILE:HB	1:F:285:THR:HG23	1.82	0.60
1:E:189:ASP:OD2	4:E:2566:HOH:O	2.16	0.60
1:C:225:ARG:NH1	1:C:275:GLU:OE2	2.34	0.60
1:C:278:VAL:CG1	1:C:305:VAL:HG21	2.20	0.60
1:C:280:ILE:HD11	1:C:313:ILE:HB	1.82	0.60
1:D:242:ILE:HD12	1:D:285:THR:HG23	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:144:ILE:CD1	1:F:291:ILE:CD1	2.70	0.60
1:F:117:ARG:HG2	1:F:118:THR:H	1.66	0.60
1:C:244:GLU:HG2	1:C:276:PHE:CD1	2.36	0.60
1:B:87:ASN:ND2	1:B:89:SER:H	1.99	0.60
1:D:258:ASN:ND2	1:D:259:GLU:H	2.00	0.59
1:D:170:VAL:H	1:D:204:ASN:HD21	1.50	0.59
1:D:19:ALA:HB2	1:D:39:VAL:CG1	2.32	0.59
1:F:211:THR:HG22	1:F:212:GLY:N	2.17	0.59
1:B:280:ILE:HD12	1:B:313:ILE:HB	1.84	0.59
1:F:113:THR:HG23	1:F:117:ARG:HD2	1.84	0.59
1:A:211:THR:CG2	1:A:212:GLY:N	2.66	0.59
1:C:19:ALA:HB2	1:C:39:VAL:HG12	1.83	0.59
1:A:87:ASN:ND2	1:A:89:SER:H	2.01	0.59
1:A:162:LYS:HE2	1:A:162:LYS:HA	1.85	0.58
1:A:13:GLU:HG3	4:A:2647:HOH:O	2.03	0.58
1:A:280:ILE:HD11	1:A:313:ILE:HB	1.85	0.58
1:D:135:CYS:O	1:D:144:ILE:HD11	2.02	0.58
1:A:13:GLU:N	4:A:2618:HOH:O	2.37	0.58
1:E:87:ASN:HD22	1:E:89:SER:H	1.51	0.58
1:B:141:GLY:HA2	1:C:291:ILE:HG21	1.86	0.58
1:A:211:THR:HG23	1:A:302:GLN:CD	2.24	0.58
1:D:117:ARG:HG2	1:D:118:THR:N	2.17	0.57
1:F:304:LYS:HB3	1:F:304:LYS:NZ	2.19	0.57
1:D:278:VAL:CG1	1:D:305:VAL:HG11	2.34	0.57
1:F:258:ASN:ND2	1:F:259:GLU:H	1.99	0.57
1:F:242:ILE:HD12	1:F:285:THR:HG23	1.87	0.57
1:F:158:GLU:H	1:F:158:GLU:CD	2.07	0.57
1:C:226:MET:HE1	1:C:241:VAL:HG21	1.86	0.57
1:A:256:LEU:H	1:B:258:ASN:ND2	2.02	0.57
1:C:289:HIS:C	1:C:291:ILE:N	2.56	0.57
1:F:225:ARG:CG	1:F:275:GLU:HG2	2.34	0.57
1:D:13:GLU:HG3	4:D:2604:HOH:O	2.04	0.57
1:F:19:ALA:HB2	1:F:39:VAL:CG1	2.34	0.57
1:C:158:GLU:CD	1:C:158:GLU:H	2.07	0.57
1:D:244:GLU:HG2	1:D:276:PHE:CD1	2.40	0.56
1:A:248:LYS:HE3	1:A:275:GLU:OE1	2.05	0.56
1:A:19:ALA:HB2	1:A:39:VAL:HG12	1.88	0.56
1:D:30:ALA:HA	1:D:73:ARG:CZ	2.36	0.56
1:B:19:ALA:HB2	1:B:39:VAL:HG12	1.87	0.56
1:A:19:ALA:HB2	1:A:39:VAL:CG1	2.35	0.56
1:B:127:GLN:HE21	1:C:260:ASN:HD22	1.54	0.56
1:B:211:THR:CG2	1:B:212:GLY:N	2.68	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:127:GLN:HE21	1:F:260:ASN:HD22	1.53	0.56
1:D:306:GLU:HG3	4:D:2662:HOH:O	2.06	0.56
1:C:278:VAL:CG1	1:C:305:VAL:HG11	2.36	0.55
1:A:256:LEU:H	1:B:258:ASN:HD21	1.52	0.55
1:F:278:VAL:CG1	1:F:305:VAL:HG21	2.26	0.55
1:A:241:VAL:HG22	1:A:286:LEU:HD22	1.89	0.55
1:A:278:VAL:HG12	1:A:278:VAL:O	2.06	0.55
1:B:290:SER:HB2	1:B:293:ARG:HD2	1.87	0.55
1:B:33:ARG:NH2	1:B:78:ASP:OD2	2.39	0.55
1:A:92:VAL:HG12	4:A:2558:HOH:O	2.06	0.55
1:C:280:ILE:HD12	1:C:313:ILE:HB	1.87	0.55
1:C:19:ALA:HB2	1:C:39:VAL:CG1	2.36	0.55
1:D:278:VAL:HG12	1:D:305:VAL:HG11	1.88	0.55
1:B:13:GLU:HG3	1:B:14:LEU:N	2.22	0.55
1:D:43:MET:HE1	1:D:98:PHE:HZ	1.72	0.55
1:D:87:ASN:ND2	1:D:89:SER:H	2.05	0.54
1:A:23:HIS:CE1	4:A:2538:HOH:O	2.60	0.54
1:C:170:VAL:H	1:C:204:ASN:ND2	2.05	0.54
1:E:31:ILE:CG2	1:E:33:ARG:HG3	2.38	0.54
1:D:260:ASN:HD22	1:F:127:GLN:HE21	1.56	0.54
1:F:170:VAL:H	1:F:204:ASN:ND2	2.05	0.54
1:D:19:ALA:HB2	1:D:39:VAL:HG12	1.90	0.54
1:E:258:ASN:ND2	1:E:259:GLU:H	2.06	0.54
1:F:13:GLU:O	1:F:14:LEU:O	2.26	0.54
1:D:225:ARG:CG	1:D:275:GLU:HG2	2.37	0.54
1:A:244:GLU:HG2	1:A:276:PHE:CD1	2.43	0.54
1:B:304:LYS:HB3	1:B:304:LYS:NZ	2.23	0.54
1:C:280:ILE:HG13	1:C:313:ILE:HD12	1.89	0.54
1:F:13:GLU:HA	4:F:2551:HOH:O	2.08	0.54
1:A:278:VAL:HG12	1:A:305:VAL:HG11	1.89	0.53
1:D:34:ASP:HB2	4:D:2734:HOH:O	2.07	0.53
1:D:44:GLU:HA	1:D:85:SER:O	2.08	0.53
1:D:158:GLU:CD	1:D:158:GLU:H	2.10	0.53
1:D:226:MET:HE1	1:D:241:VAL:HG21	1.90	0.53
1:A:289:HIS:C	1:A:291:ILE:N	2.61	0.53
1:C:211:THR:CG2	1:C:212:GLY:N	2.71	0.53
1:A:158:GLU:CD	1:A:158:GLU:H	2.12	0.53
1:C:278:VAL:HG12	1:C:305:VAL:HG11	1.91	0.53
1:C:258:ASN:ND2	1:C:259:GLU:H	2.02	0.53
1:F:31:ILE:HG23	1:F:33:ARG:HG3	1.89	0.53
1:A:26:GLU:HG3	4:A:2784:HOH:O	2.08	0.53
1:C:306:GLU:HG3	4:C:2600:HOH:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:225:ARG:CG	1:E:275:GLU:HG2	2.38	0.53
1:B:279:ASP:N	1:B:279:ASP:OD2	2.38	0.52
1:C:290:SER:HB2	1:C:293:ARG:HD2	1.92	0.52
1:E:33:ARG:NH2	1:E:78:ASP:OD2	2.42	0.52
1:C:55:GLY:HA3	1:C:183:GLN:NE2	2.24	0.52
1:C:225:ARG:HG3	1:C:275:GLU:HG2	1.91	0.52
1:A:23:HIS:HE1	4:A:2538:HOH:O	1.93	0.52
1:F:226:MET:HE1	1:F:276:PHE:HE2	1.74	0.52
1:F:244:GLU:HG2	1:F:276:PHE:CD1	2.45	0.52
1:E:211:THR:CG2	1:E:212:GLY:N	2.71	0.52
1:B:43:MET:HE2	1:B:98:PHE:HZ	1.74	0.52
1:B:158:GLU:H	1:B:158:GLU:CD	2.12	0.52
1:B:95:ASN:HB3	1:B:112:PHE:HA	1.92	0.51
1:F:226:MET:CE	1:F:276:PHE:HE2	2.23	0.51
1:A:70:ARG:CZ	4:A:2562:HOH:O	2.58	0.51
1:B:175:TYR:CD1	1:B:175:TYR:N	2.78	0.51
1:C:25:PRO:HD2	1:C:26:GLU:H	1.75	0.51
1:E:289:HIS:C	1:E:291:ILE:H	2.13	0.51
1:A:280:ILE:HD12	1:A:313:ILE:HB	1.91	0.51
1:A:30:ALA:HA	1:A:73:ARG:CZ	2.41	0.51
1:A:33:ARG:NH2	1:A:78:ASP:OD2	2.41	0.51
1:D:13:GLU:HA	4:D:2747:HOH:O	2.10	0.51
1:B:33:ARG:HH22	1:B:78:ASP:CG	2.14	0.51
1:A:33:ARG:HH22	1:A:78:ASP:CG	2.13	0.51
1:E:34:ASP:HB2	4:E:2711:HOH:O	2.11	0.51
1:D:264:THR:CG2	1:F:252:GLU:OE1	2.59	0.51
1:C:278:VAL:O	1:C:278:VAL:HG12	2.11	0.50
1:E:95:ASN:HB3	1:E:112:PHE:HA	1.92	0.50
1:D:144:ILE:HD12	1:D:144:ILE:N	2.27	0.50
1:A:127:GLN:HE21	1:B:260:ASN:ND2	2.08	0.50
1:D:127:GLN:HE21	1:E:260:ASN:ND2	2.07	0.50
1:D:286:LEU:N	1:D:286:LEU:HD23	2.27	0.50
1:A:258:ASN:ND2	1:A:259:GLU:H	2.08	0.50
1:B:173:ASP:OD1	1:B:233:PRO:HD2	2.11	0.50
1:B:112:PHE:O	1:B:117:ARG:NH1	2.45	0.49
1:F:87:ASN:ND2	1:F:89:SER:H	2.08	0.49
1:B:33:ARG:N	4:B:594:HOH:O	2.45	0.49
1:D:21:THR:OG1	1:D:70:ARG:HD3	2.12	0.49
1:A:112:PHE:O	1:A:117:ARG:NH1	2.45	0.49
1:D:34:ASP:CG	4:D:2600:HOH:O	2.49	0.49
1:A:264:THR:CG2	1:C:252:GLU:OE1	2.60	0.49
1:C:211:THR:HG23	1:C:302:GLN:CD	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:289:HIS:O	1:C:291:ILE:N	2.45	0.49
1:E:54:ASP:HB2	4:E:2734:HOH:O	2.11	0.49
1:F:226:MET:HE1	1:F:241:VAL:HG21	1.93	0.49
1:B:289:HIS:C	1:B:291:ILE:N	2.64	0.49
1:D:256:LEU:H	1:E:258:ASN:ND2	2.11	0.49
1:D:258:ASN:ND2	1:F:256:LEU:H	2.10	0.49
1:A:258:ASN:HD22	1:A:259:GLU:N	2.10	0.49
1:D:260:ASN:ND2	1:F:127:GLN:HE21	2.10	0.49
1:D:286:LEU:H	1:D:286:LEU:HD23	1.77	0.49
1:C:13:GLU:N	4:C:2684:HOH:O	2.45	0.49
1:A:278:VAL:HG11	1:A:305:VAL:HG11	1.94	0.49
1:B:226:MET:CE	1:B:276:PHE:HE2	2.26	0.49
1:F:211:THR:HG23	1:F:302:GLN:CD	2.33	0.49
1:D:258:ASN:HD22	1:D:259:GLU:N	2.06	0.49
1:B:175:TYR:CD2	1:B:193:ALA:HA	2.48	0.49
1:A:258:ASN:ND2	1:C:256:LEU:H	2.11	0.48
1:D:92:VAL:HB	4:D:2852:HOH:O	2.12	0.48
1:E:31:ILE:HD11	1:E:74:VAL:HA	1.95	0.48
1:A:291:ILE:HG21	1:C:141:GLY:HA2	1.95	0.48
1:B:170:VAL:H	1:B:204:ASN:ND2	2.10	0.48
1:A:280:ILE:HD11	1:A:310:ASN:O	2.12	0.48
1:E:226:MET:HE2	1:E:276:PHE:HE2	1.77	0.48
1:D:291:ILE:HG21	1:F:141:GLY:HA2	1.94	0.48
1:A:225:ARG:CG	1:A:275:GLU:HG2	2.39	0.48
1:E:304:LYS:NZ	1:E:304:LYS:HB3	2.28	0.48
1:C:180:LYS:HD2	4:C:2797:HOH:O	2.13	0.48
1:E:141:GLY:HA2	1:F:291:ILE:HG21	1.94	0.48
1:E:286:LEU:HD23	1:E:286:LEU:N	2.27	0.48
1:F:173:ASP:OD1	1:F:233:PRO:HD2	2.13	0.48
1:D:252:GLU:OE1	1:E:264:THR:CG2	2.55	0.48
1:F:289:HIS:C	1:F:291:ILE:N	2.67	0.48
1:D:211:THR:CG2	1:D:212:GLY:H	2.27	0.48
1:D:291:ILE:CG2	1:D:292:PHE:N	2.77	0.48
1:B:226:MET:HE1	1:B:241:VAL:HG21	1.95	0.48
1:A:250:TYR:HB2	1:A:273:ILE:HB	1.96	0.48
1:E:87:ASN:ND2	1:E:89:SER:H	2.10	0.48
1:A:117:ARG:HG2	1:A:118:THR:H	1.76	0.48
1:F:242:ILE:HD12	1:F:285:THR:CG2	2.44	0.48
1:C:95:ASN:HB3	1:C:112:PHE:HA	1.95	0.48
1:A:242:ILE:HB	1:A:285:THR:HG23	1.96	0.48
1:F:211:THR:CG2	1:F:212:GLY:N	2.77	0.47
1:F:180:LYS:NZ	4:F:2600:HOH:O	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:127:GLN:HE21	1:C:260:ASN:ND2	2.11	0.47
1:E:127:GLN:HE21	1:F:260:ASN:ND2	2.12	0.47
1:F:31:ILE:HG22	1:F:33:ARG:HG3	1.95	0.47
1:A:170:VAL:H	1:A:204:ASN:ND2	2.12	0.47
1:D:289:HIS:C	1:D:291:ILE:N	2.67	0.47
1:F:292:PHE:O	1:F:296:ASN:HB2	2.14	0.47
1:D:314:MET:HG3	1:F:102:THR:O	2.14	0.47
1:B:211:THR:HG23	1:B:302:GLN:OE1	2.14	0.47
1:C:17:ILE:HD11	4:C:2558:HOH:O	2.14	0.47
1:D:256:LEU:HB2	1:E:258:ASN:ND2	2.30	0.47
1:D:225:ARG:NH1	1:D:275:GLU:OE2	2.48	0.47
1:A:256:LEU:HD21	1:B:256:LEU:HG	1.97	0.47
1:B:44:GLU:HA	1:B:85:SER:O	2.14	0.47
1:D:211:THR:HG23	1:D:302:GLN:OE1	2.15	0.47
1:E:211:THR:HG23	1:E:302:GLN:CD	2.35	0.47
1:A:25:PRO:HD2	1:A:26:GLU:H	1.80	0.47
1:D:70:ARG:NE	4:D:2603:HOH:O	2.46	0.47
1:C:310:ASN:OD1	1:C:312:GLU:HB2	2.14	0.47
1:E:190:MET:HG3	4:E:2720:HOH:O	2.15	0.47
1:E:261:VAL:HG11	1:E:264:THR:HG23	1.97	0.46
1:D:70:ARG:NH2	4:D:2603:HOH:O	2.47	0.46
1:F:204:ASN:OD1	1:F:210:LEU:HD21	2.15	0.46
1:D:33:ARG:NH2	1:D:78:ASP:OD2	2.48	0.46
1:B:117:ARG:HG3	4:B:693:HOH:O	2.15	0.46
1:D:162:LYS:HA	1:D:162:LYS:HE2	1.96	0.46
1:C:242:ILE:HD12	1:C:285:THR:HG23	1.96	0.46
1:E:31:ILE:HG23	1:E:33:ARG:HG3	1.97	0.46
1:C:280:ILE:HD11	1:C:310:ASN:HB3	1.97	0.46
1:E:211:THR:HG23	1:E:302:GLN:OE1	2.15	0.46
1:E:117:ARG:HG3	4:E:2792:HOH:O	2.15	0.46
1:D:256:LEU:H	1:E:258:ASN:HD21	1.63	0.46
1:A:21:THR:OG1	1:A:70:ARG:HD3	2.16	0.46
1:B:250:TYR:HB2	1:B:273:ILE:HB	1.97	0.46
1:F:278:VAL:HG11	1:F:305:VAL:HG11	1.96	0.46
1:B:31:ILE:CG2	1:B:33:ARG:HG3	2.46	0.46
1:E:217:LYS:HE2	1:E:304:LYS:HD3	1.96	0.46
1:F:277:LYS:HE2	1:F:279:ASP:HB3	1.97	0.46
1:A:225:ARG:NH1	1:A:275:GLU:OE2	2.49	0.46
1:C:226:MET:CE	1:C:276:PHE:HE2	2.28	0.46
1:E:226:MET:HE1	1:E:241:VAL:HG21	1.98	0.45
1:A:313:ILE:O	1:C:123:PHE:HA	2.16	0.45
1:E:51:LYS:HE3	1:E:54:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:44:GLU:HA	1:F:85:SER:O	2.16	0.45
1:E:23:HIS:CE1	4:E:2567:HOH:O	2.69	0.45
1:E:258:ASN:HD22	1:E:259:GLU:N	2.13	0.45
1:C:226:MET:HE2	1:C:276:PHE:HE2	1.82	0.45
1:F:43:MET:HE1	1:F:98:PHE:HZ	1.81	0.45
1:D:129:GLY:HA2	4:D:2659:HOH:O	2.16	0.45
1:E:43:MET:HE2	1:E:98:PHE:HZ	1.81	0.45
1:E:44:GLU:HA	1:E:85:SER:O	2.17	0.45
1:F:286:LEU:HD23	1:F:286:LEU:N	2.32	0.45
1:B:51:LYS:HE2	1:B:54:ASP:HA	1.98	0.45
1:C:249:VAL:HG11	1:C:264:THR:CG2	2.39	0.45
1:B:219:LYS:O	1:B:222:GLU:HG3	2.16	0.45
1:A:211:THR:CG2	1:A:212:GLY:H	2.30	0.45
1:C:31:ILE:HG23	1:C:33:ARG:HG3	1.97	0.45
1:B:165:LYS:HD2	1:B:222:GLU:OE2	2.16	0.45
1:F:281:PRO:HG2	1:F:307:GLY:C	2.37	0.45
1:A:277:LYS:HE2	1:A:279:ASP:HB3	1.98	0.45
1:F:14:LEU:N	4:F:2551:HOH:O	2.50	0.44
1:A:292:PHE:O	1:A:296:ASN:HB2	2.17	0.44
1:B:175:TYR:CE2	1:B:193:ALA:HA	2.51	0.44
1:E:32:ASP:C	4:E:2585:HOH:O	2.55	0.44
1:E:19:ALA:HB2	1:E:39:VAL:HG12	1.98	0.44
1:C:31:ILE:HG23	1:C:33:ARG:CG	2.48	0.44
1:D:292:PHE:O	1:D:296:ASN:HB2	2.16	0.44
1:B:225:ARG:HH11	1:B:225:ARG:HG3	1.82	0.44
1:E:250:TYR:HB2	1:E:273:ILE:HB	2.00	0.44
1:D:43:MET:HE3	1:D:96:VAL:HG11	2.00	0.44
1:A:278:VAL:CG1	1:A:305:VAL:HG21	2.36	0.44
1:A:226:MET:CE	1:A:276:PHE:HE2	2.31	0.44
1:D:211:THR:HG21	4:D:2814:HOH:O	2.18	0.44
1:B:211:THR:HG23	1:B:302:GLN:CD	2.38	0.44
1:C:43:MET:CE	1:C:82:VAL:HG11	2.47	0.44
1:F:95:ASN:HB3	1:F:112:PHE:HA	2.00	0.44
1:D:210:LEU:HD22	1:D:216:LEU:HD21	2.00	0.44
1:A:70:ARG:NE	4:A:2562:HOH:O	2.50	0.44
1:F:51:LYS:HE3	1:F:54:ASP:HA	2.00	0.44
1:E:158:GLU:H	1:E:158:GLU:CD	2.21	0.44
1:E:170:VAL:H	1:E:204:ASN:ND2	2.16	0.44
1:D:310:ASN:OD1	1:D:312:GLU:HB2	2.18	0.43
1:C:304:LYS:NZ	1:C:304:LYS:HB3	2.32	0.43
1:E:249:VAL:CG1	1:E:264:THR:HG21	2.30	0.43
1:A:280:ILE:HA	1:A:281:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:291:ILE:HG22	1:D:292:PHE:N	2.32	0.43
1:C:250:TYR:HB2	1:C:273:ILE:HB	2.00	0.43
1:F:179:LYS:HE2	4:F:2765:HOH:O	2.18	0.43
1:D:175:TYR:CD1	1:D:175:TYR:N	2.86	0.43
1:F:236:VAL:CG1	1:F:265:ILE:HG23	2.48	0.43
1:E:175:TYR:CD1	1:E:175:TYR:N	2.86	0.43
1:A:186:GLN:HA	1:A:187:PRO:HD3	1.87	0.43
1:F:13:GLU:CD	1:F:38:LYS:NZ	2.72	0.43
1:C:170:VAL:H	1:C:204:ASN:HD21	1.67	0.43
1:C:180:LYS:HG2	1:C:200:TYR:CE2	2.53	0.43
1:E:16:VAL:HG11	1:E:40:ARG:NE	2.34	0.43
1:F:280:ILE:HA	1:F:281:PRO:HD3	1.89	0.43
1:A:211:THR:HG23	1:A:302:GLN:OE1	2.19	0.43
1:E:112:PHE:O	1:E:117:ARG:NH1	2.52	0.43
1:E:33:ARG:HH22	1:E:78:ASP:CG	2.20	0.43
1:D:162:LYS:HE3	4:D:2583:HOH:O	2.18	0.43
1:F:43:MET:CE	1:F:82:VAL:HG11	2.48	0.43
1:B:278:VAL:CG1	1:B:305:VAL:HG21	2.24	0.43
1:D:280:ILE:HA	1:D:281:PRO:HD3	1.89	0.43
1:D:225:ARG:HH11	1:D:225:ARG:HG3	1.84	0.43
1:B:186:GLN:HA	1:B:187:PRO:HD3	1.90	0.42
1:A:310:ASN:OD1	1:A:312:GLU:HB2	2.19	0.42
1:D:27:VAL:HG13	1:D:71:MET:CE	2.49	0.42
1:B:226:MET:HE3	1:B:239:PHE:HE2	1.83	0.42
1:C:211:THR:HG23	1:C:302:GLN:OE1	2.18	0.42
1:A:291:ILE:HG22	1:A:292:PHE:N	2.35	0.42
1:D:114:ALA:H	1:D:117:ARG:HD2	1.85	0.42
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.91	0.42
1:E:122:SER:O	1:F:314:MET:HA	2.19	0.42
4:A:2529:HOH:O	1:B:297:LYS:HE3	2.20	0.42
1:A:289:HIS:C	1:A:291:ILE:H	2.22	0.42
1:C:13:GLU:CB	4:C:2684:HOH:O	2.67	0.42
1:E:33:ARG:HD3	4:E:2795:HOH:O	2.19	0.42
1:B:289:HIS:C	1:B:291:ILE:H	2.23	0.42
1:E:175:TYR:CD2	1:E:193:ALA:HA	2.54	0.42
1:F:97:ASP:O	1:F:133:TYR:HA	2.20	0.42
1:B:27:VAL:HG13	1:B:71:MET:SD	2.60	0.42
1:B:87:ASN:HA	1:B:88:PRO:HD3	1.95	0.42
1:A:36:PRO:HA	4:A:2568:HOH:O	2.20	0.42
1:F:176:THR:CG2	1:F:186:GLN:HB3	2.40	0.42
1:E:162:LYS:HA	1:E:162:LYS:CE	2.45	0.42
1:D:43:MET:CE	1:D:82:VAL:HG11	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:GLU:OE1	1:C:264:THR:HG22	2.20	0.42
1:F:217:LYS:HD3	1:F:304:LYS:HB2	2.01	0.42
1:D:175:TYR:CD2	1:D:193:ALA:HA	2.55	0.42
1:A:55:GLY:HA3	1:A:183:GLN:HE22	1.84	0.42
1:A:142:MET:HG3	1:A:188:PHE:CE2	2.55	0.42
1:B:280:ILE:HD13	4:B:772:HOH:O	2.20	0.41
1:E:289:HIS:O	1:E:291:ILE:N	2.44	0.41
1:C:280:ILE:HA	1:C:281:PRO:HD3	1.91	0.41
1:D:226:MET:CE	1:D:276:PHE:HE2	2.33	0.41
1:B:210:LEU:HD22	1:B:216:LEU:HD21	2.03	0.41
1:E:180:LYS:HD3	4:E:2601:HOH:O	2.19	0.41
1:D:280:ILE:HD11	1:D:310:ASN:O	2.20	0.41
1:B:25:PRO:HD2	1:B:26:GLU:H	1.84	0.41
1:B:236:VAL:CG1	1:B:265:ILE:HG23	2.49	0.41
1:E:225:ARG:NH1	1:E:275:GLU:OE2	2.52	0.41
1:A:44:GLU:HA	1:A:85:SER:O	2.20	0.41
1:D:144:ILE:CD1	1:D:144:ILE:N	2.84	0.41
1:D:304:LYS:NZ	1:D:304:LYS:HB3	2.35	0.41
1:E:280:ILE:HD13	4:E:2743:HOH:O	2.19	0.41
1:B:43:MET:HE1	1:B:96:VAL:HG11	2.03	0.41
1:A:35:TYR:HA	1:A:36:PRO:HD3	1.91	0.41
1:C:292:PHE:O	1:C:296:ASN:HB2	2.20	0.41
1:E:144:ILE:HD13	1:F:291:ILE:HD13	1.72	0.41
1:D:43:MET:HE1	1:D:98:PHE:CZ	2.53	0.41
1:F:170:VAL:H	1:F:204:ASN:HD21	1.67	0.41
1:D:186:GLN:HA	1:D:187:PRO:HD3	1.91	0.41
1:A:280:ILE:HD11	1:A:310:ASN:HB3	2.03	0.41
1:B:226:MET:HE1	1:B:276:PHE:HE2	1.86	0.41
1:F:31:ILE:HG23	1:F:33:ARG:CG	2.50	0.41
1:D:242:ILE:HD12	1:D:285:THR:CG2	2.48	0.41
1:D:226:MET:HE2	1:D:276:PHE:HE2	1.86	0.41
1:B:170:VAL:H	1:B:204:ASN:HD21	1.68	0.41
1:A:142:MET:HG3	1:A:188:PHE:CD2	2.56	0.41
1:F:55:GLY:HA3	1:F:183:GLN:HE22	1.86	0.41
1:C:279:ASP:N	1:C:279:ASP:OD2	2.41	0.41
1:D:256:LEU:HG	1:F:256:LEU:HD21	2.03	0.41
1:F:68:PRO:HD3	1:F:204:ASN:HA	2.03	0.41
1:D:291:ILE:HA	1:D:291:ILE:HD13	1.86	0.41
1:D:33:ARG:HH22	1:D:78:ASP:CG	2.25	0.41
1:C:175:TYR:CD1	1:C:175:TYR:N	2.90	0.41
1:C:87:ASN:ND2	1:C:89:SER:H	2.12	0.40
1:A:268:ALA:O	1:B:289:HIS:HB3	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:36:PRO:HA	4:F:2556:HOH:O	2.22	0.40
1:D:113:THR:HG23	1:D:117:ARG:HD2	2.03	0.40
1:E:219:LYS:O	1:E:222:GLU:HG3	2.21	0.40
1:D:279:ASP:OD2	1:D:279:ASP:N	2.51	0.40
1:D:173:ASP:OD1	1:D:233:PRO:HD2	2.21	0.40
1:D:101:ALA:HB1	1:E:314:MET:CE	2.51	0.40
1:A:260:ASN:HD22	1:C:127:GLN:HE21	1.69	0.40
1:C:33:ARG:NH2	1:C:37:ALA:HB3	2.37	0.40
1:D:87:ASN:HA	1:D:88:PRO:HD3	1.95	0.40
1:E:226:MET:HE3	1:E:239:PHE:HE2	1.86	0.40
1:B:258:ASN:HD22	1:B:259:GLU:H	1.69	0.40
1:B:13:GLU:HG3	1:B:14:LEU:H	1.86	0.40
1:D:175:TYR:CE2	1:D:193:ALA:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/327 (92%)	290 (97%)	8 (3%)	2 (1%)	30	15
1	B	300/327 (92%)	289 (96%)	9 (3%)	2 (1%)	30	15
1	C	300/327 (92%)	288 (96%)	10 (3%)	2 (1%)	30	15
1	D	300/327 (92%)	289 (96%)	9 (3%)	2 (1%)	30	15
1	E	300/327 (92%)	291 (97%)	8 (3%)	1 (0%)	50	38
1	F	300/327 (92%)	287 (96%)	10 (3%)	3 (1%)	22	9
All	All	1800/1962 (92%)	1734 (96%)	54 (3%)	12 (1%)	30	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	B	25	PRO

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Mol	Chain	Res	Type
1	C	25	PRO
1	F	14	LEU
1	F	25	PRO
1	A	291	ILE
1	B	291	ILE
1	C	291	ILE
1	E	291	ILE
1	F	291	ILE
1	D	291	ILE
1	D	205	GLY

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	239/259 (92%)	231 (97%)	8 (3%)	50	35
1	B	239/259 (92%)	228 (95%)	11 (5%)	37	20
1	C	239/259 (92%)	229 (96%)	10 (4%)	40	24
1	D	239/259 (92%)	228 (95%)	11 (5%)	37	20
1	E	239/259 (92%)	231 (97%)	8 (3%)	50	35
1	F	239/259 (92%)	230 (96%)	9 (4%)	44	29
All	All	1434/1554 (92%)	1377 (96%)	57 (4%)	42	26

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	121	PHE
1	A	173	ASP
1	A	258	ASN
1	A	264	THR
1	A	285	THR
1	A	290	SER
1	A	291	ILE
1	B	33	ARG

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Mol	Chain	Res	Type
1	B	121	PHE
1	B	158	GLU
1	B	173	ASP
1	B	180	LYS
1	B	258	ASN
1	B	264	THR
1	B	279	ASP
1	B	285	THR
1	B	286	LEU
1	B	291	ILE
1	C	33	ARG
1	C	121	PHE
1	C	158	GLU
1	C	173	ASP
1	C	258	ASN
1	C	264	THR
1	C	279	ASP
1	C	285	THR
1	C	286	LEU
1	C	291	ILE
1	D	33	ARG
1	D	46	VAL
1	D	121	PHE
1	D	173	ASP
1	D	258	ASN
1	D	264	THR
1	D	279	ASP
1	D	285	THR
1	D	286	LEU
1	D	291	ILE
1	D	314	MET
1	E	33	ARG
1	E	121	PHE
1	E	173	ASP
1	E	258	ASN
1	E	264	THR
1	E	285	THR
1	E	286	LEU
1	E	291	ILE
1	F	33	ARG
1	F	46	VAL
1	F	121	PHE

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Mol	Chain	Res	Type
1	F	173	ASP
1	F	258	ASN
1	F	264	THR
1	F	279	ASP
1	F	285	THR
1	F	286	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	87	ASN
1	A	183	GLN
1	A	197	GLN
1	A	204	ASN
1	A	258	ASN
1	B	87	ASN
1	B	183	GLN
1	B	204	ASN
1	B	258	ASN
1	B	260	ASN
1	C	87	ASN
1	C	127	GLN
1	C	183	GLN
1	C	204	ASN
1	C	258	ASN
1	C	260	ASN
1	C	296	ASN
1	D	23	HIS
1	D	87	ASN
1	D	183	GLN
1	D	204	ASN
1	D	258	ASN
1	D	260	ASN
1	E	87	ASN
1	E	258	ASN
1	E	260	ASN
1	F	87	ASN
1	F	183	GLN
1	F	204	ASN
1	F	258	ASN
1	F	260	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NO2	A	2504	2	2,2,2	1.63	0	1,1,1	0.35	0
3	NO2	A	2506	2	2,2,2	1.60	0	1,1,1	0.36	0
3	NO2	C	2505	2	2,2,2	1.62	0	1,1,1	0.34	0
3	NO2	D	2509	2	2,2,2	1.65	0	1,1,1	0.34	0
3	NO2	E	2507	2	2,2,2	1.64	0	1,1,1	0.34	0
3	NO2	F	2508	2	2,2,2	1.61	0	1,1,1	0.34	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
3	NO2	A	2504	2	-	0/0/0/0	0/0/0/0
3	NO2	A	2506	2	-	0/0/0/0	0/0/0/0
3	NO2	C	2505	2	-	0/0/0/0	0/0/0/0
3	NO2	D	2509	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NO2	E	2507	2	-	0/0/0/0	0/0/0/0
3	NO2	F	2508	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	302/327 (92%)	-0.01	10 (3%) 44 51	12, 20, 35, 59	0
1	B	302/327 (92%)	-0.05	7 (2%) 57 65	12, 21, 33, 51	0
1	C	302/327 (92%)	0.04	7 (2%) 57 65	13, 23, 38, 55	0
1	D	302/327 (92%)	-0.02	8 (2%) 53 61	12, 20, 36, 55	0
1	E	302/327 (92%)	0.06	12 (3%) 36 41	12, 23, 36, 49	0
1	F	302/327 (92%)	0.13	11 (3%) 41 47	13, 22, 37, 58	0
All	All	1812/1962 (92%)	0.03	55 (3%) 48 55	12, 22, 36, 59	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	13	GLU	6.2
1	F	308	ALA	5.4
1	A	308	ALA	4.8
1	F	307	GLY	3.9
1	E	307	GLY	3.8
1	F	311	PRO	3.6
1	F	32	ASP	3.6
1	E	308	ALA	3.5
1	C	13	GLU	3.3
1	F	309	GLU	3.2
1	B	32	ASP	3.2
1	A	280	ILE	3.2
1	D	308	ALA	3.1
1	C	34	ASP	3.1
1	C	280	ILE	3.1
1	E	117	ARG	3.1
1	B	309	GLU	2.9
1	C	307	GLY	2.9
1	D	280	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	2.9
1	D	309	GLU	2.9
1	E	309	GLU	2.9
1	C	308	ALA	2.9
1	A	311	PRO	2.8
1	E	54	ASP	2.7
1	B	117	ARG	2.7
1	F	34	ASP	2.7
1	D	314	MET	2.6
1	E	313	ILE	2.6
1	A	306	GLU	2.6
1	F	310	ASN	2.6
1	A	307	GLY	2.5
1	A	310	ASN	2.5
1	C	309	GLU	2.4
1	A	117	ARG	2.4
1	D	311	PRO	2.4
1	B	308	ALA	2.3
1	D	278	VAL	2.3
1	A	291	ILE	2.3
1	D	306	GLU	2.3
1	E	306	GLU	2.3
1	B	221	GLY	2.2
1	A	313	ILE	2.2
1	F	291	ILE	2.2
1	E	278	VAL	2.2
1	B	34	ASP	2.2
1	E	291	ILE	2.1
1	D	307	GLY	2.1
1	F	236	VAL	2.1
1	E	34	ASP	2.1
1	B	306	GLU	2.1
1	C	32	ASP	2.1
1	E	220	ALA	2.0
1	E	280	ILE	2.0
1	F	313	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q < 0.9
3	NO2	F	2508	3/3	0.17	5.31	31,31,34,35	0
3	NO2	C	2505	3/3	0.18	3.08	32,32,35,35	0
3	NO2	A	2504	3/3	0.17	2.24	32,32,33,35	0
3	NO2	E	2507	3/3	0.19	2.13	30,30,33,35	0
3	NO2	A	2506	3/3	0.18	1.44	27,27,32,33	0
3	NO2	D	2509	3/3	0.16	1.06	26,26,29,32	0
2	CU	E	501	1/1	0.04	-2.60	25,25,25,25	0
2	CU	F	501	1/1	0.03	-2.78	22,22,22,22	0
2	CU	A	501	1/1	0.03	-2.81	20,20,20,20	0
2	CU	B	501	1/1	0.03	-2.91	22,22,22,22	0
2	CU	D	502	1/1	0.03	-3.08	23,23,23,23	0
2	CU	A	502	1/1	0.03	-3.29	21,21,21,21	0
2	CU	C	502	1/1	0.04	-3.37	23,23,23,23	0
2	CU	D	501	1/1	0.03	-3.89	20,20,20,20	0
2	CU	E	502	1/1	0.03	-4.43	25,25,25,25	0
2	CU	B	502	1/1	0.03	-4.68	24,24,24,24	0
2	CU	F	502	1/1	0.03	-5.02	24,24,24,24	0
2	CU	C	501	1/1	0.02	-5.24	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.