



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:47 PM EST

PDB ID : 1NLX
Title : Crystal Structure of PHL P 6, A Major Timothy Grass Pollen Allergen Co-Crystallized with Zinc
Authors : Fedorov, A.A.; Ball, T.; Fedorov, E.V.; Vrtala, S.; Valenta, R.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYS-GXRC)
Deposited on : 2003-01-07
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.16
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

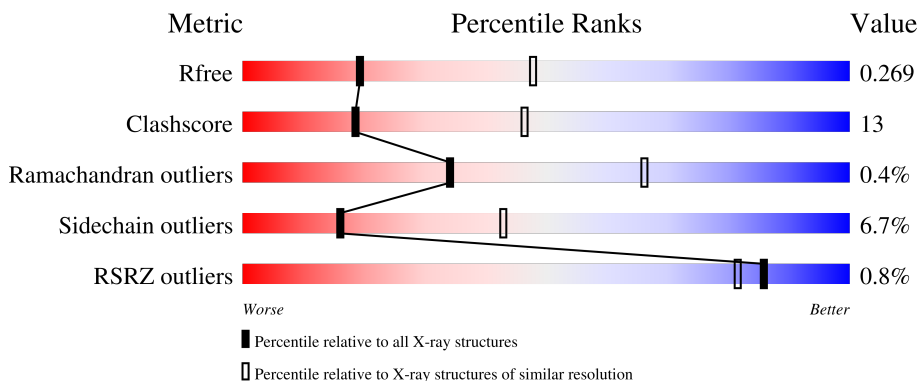
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	111	
1	B	111	
1	C	111	
1	D	111	
1	E	111	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	111	 68% 24% • 6%
1	G	111	 70% 20% • 6%
1	H	111	 70% 22% • 6%
1	I	111	 73% 18% • 6%
1	J	111	 73% 17% • 6%
1	K	111	 70% 20% • 6%
1	L	111	 70% 21% • 6%
1	M	111	 69% 21% • 6%
1	N	111	 71% 20% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11151 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 Pollen allergen Phl p 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	104	794	503	133	157	1	0	0	0
1	B	104	794	503	133	157	1	0	0	0
1	C	104	794	503	133	157	1	0	0	0
1	D	104	794	503	133	157	1	0	0	0
1	E	104	794	503	133	157	1	0	0	0
1	F	104	794	503	133	157	1	0	0	0
1	G	104	794	503	133	157	1	0	0	0
1	H	104	794	503	133	157	1	0	0	0
1	I	104	794	503	133	157	1	0	0	0
1	J	104	794	503	133	157	1	0	0	0
1	K	104	794	503	133	157	1	0	0	0
1	L	104	794	503	133	157	1	0	0	0
1	M	104	794	503	133	157	1	0	0	0
1	N	104	794	503	133	157	1	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	MET	-	cloning artifact	UNP P43215

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	601	MET	-	cloning artifact	UNP P43215
C	801	MET	-	cloning artifact	UNP P43215
D	1001	MET	-	cloning artifact	UNP P43215
E	1201	MET	-	cloning artifact	UNP P43215
F	1401	MET	-	cloning artifact	UNP P43215
G	1601	MET	-	cloning artifact	UNP P43215
H	1801	MET	-	cloning artifact	UNP P43215
I	2001	MET	-	cloning artifact	UNP P43215
J	2201	MET	-	cloning artifact	UNP P43215
K	2401	MET	-	cloning artifact	UNP P43215
L	2601	MET	-	cloning artifact	UNP P43215
M	2801	MET	-	cloning artifact	UNP P43215
N	3001	MET	-	cloning artifact	UNP P43215

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	N	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	As	0	0
			1	1		
3	K	1	Total	As	0	0
			1	1		
3	B	1	Total	As	0	0
			1	1		
3	I	1	Total	As	0	0
			1	1		
3	C	1	Total	As	0	0
			1	1		
3	N	1	Total	As	0	0
			1	1		
3	L	1	Total	As	0	0
			1	1		

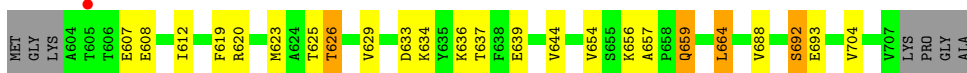
3 Residue-property plots [i](#)

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.

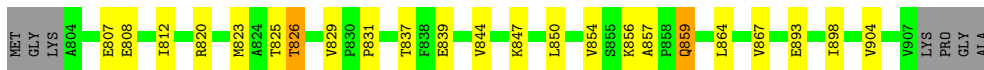
- Molecule 1: Pollen allergen Phl p 6



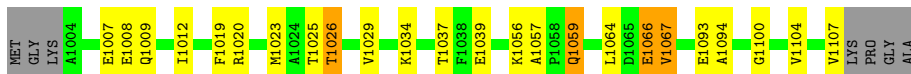
- Molecule 1: Pollen allergen Phl p 6



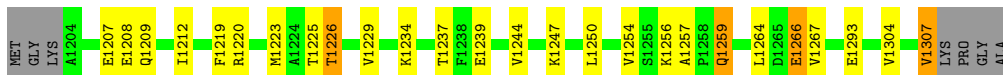
- Molecule 1: Pollen allergen Phl p 6



- Molecule 1: Pollen allergen Phl p 6



- Molecule 1: Pollen allergen Phl p 6



- Molecule 1: Pollen allergen Phl p 6

Chain F:  68% 24% 6%



• Molecule 1: Pollen allergen Phl p 6

Chain G:  70% 20% 6%



• Molecule 1: Pollen allergen Phl p 6

Chain H:  2% 70% 22% 6%



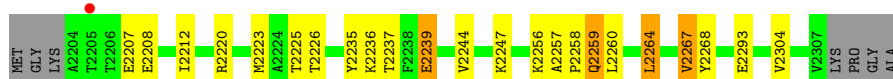
• Molecule 1: Pollen allergen Phl p 6

Chain I:  73% 18% 6%



• Molecule 1: Pollen allergen Phl p 6

Chain J:  73% 17% 6%



• Molecule 1: Pollen allergen Phl p 6

Chain K:  2% 70% 20% 6%



• Molecule 1: Pollen allergen Phl p 6

Chain L:  3% 70% 21% 6%



- Molecule 1: Pollen allergen Phl p 6

Chain M:  69% 21% • 6%



- Molecule 1: Pollen allergen Phl p 6

Chain N:  71% 20% • 6%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.81Å 110.33Å 159.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 94.3 (19.93-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.272 0.239 , 0.269	Depositor DCC
R_{free} test set	2310 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -2.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.450 for k,h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11151	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/811	0.60	0/1106
1	B	0.42	0/811	0.60	0/1106
1	C	0.43	0/811	0.59	0/1106
1	D	0.45	0/811	0.61	0/1106
1	E	0.43	0/811	0.60	0/1106
1	F	0.43	0/811	0.60	0/1106
1	G	0.43	0/811	0.60	0/1106
1	H	0.41	0/811	0.57	0/1106
1	I	0.41	0/811	0.62	0/1106
1	J	0.44	0/811	0.60	0/1106
1	K	0.42	0/811	0.63	0/1106
1	L	0.44	0/811	0.58	0/1106
1	M	0.43	0/811	0.60	0/1106
1	N	0.40	0/811	0.58	0/1106
All	All	0.42	0/11354	0.60	0/15484

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	794	0	773	23	0
1	B	794	0	773	18	0
1	C	794	0	773	16	0
1	D	794	0	773	23	0
1	E	794	0	773	23	0
1	F	794	0	773	27	0
1	G	794	0	773	30	0
1	H	794	0	773	26	0
1	I	794	0	773	25	0
1	J	794	0	773	21	0
1	K	794	0	773	26	0
1	L	794	0	773	24	0
1	M	794	0	773	33	0
1	N	794	0	773	24	0
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
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
All	All	11151	0	10822	290	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 13.

All (290) 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:G:1609:GLN:HE22	1:L:2644:VAL:HA	1.11	1.12
1:E:1220:ARG:HD3	1:E:1223:MET:HE3	1.35	1.07
1:F:1420:ARG:HD3	1:F:1423:MET:HE3	1.36	1.06
1:B:620:ARG:HD3	1:B:623:MET:HE3	1.38	1.06
1:K:2420:ARG:HD3	1:K:2423:MET:HE3	1.39	1.05
1:N:3020:ARG:HD3	1:N:3023:MET:HE3	1.41	1.02
1:M:2820:ARG:HD3	1:M:2823:MET:HE3	1.40	1.02
1:G:1620:ARG:HD3	1:G:1623:MET:HE3	1.41	1.02
1:J:2244:VAL:HA	1:M:2809:GLN:HE22	1.22	1.02
1:I:2020:ARG:HD3	1:I:2023:MET:HE3	1.40	1.02
1:L:2620:ARG:HD3	1:L:2623:MET:HE3	1.42	1.01
1:C:820:ARG:HD3	1:C:823:MET:HE3	1.42	1.01
1:D:1020:ARG:HD3	1:D:1023:MET:HE3	1.39	1.00
1:A:420:ARG:HD3	1:A:423:MET:HE3	1.44	0.99
1:J:2220:ARG:HD3	1:J:2223:MET:HE3	1.44	0.99
1:H:1820:ARG:HD3	1:H:1823:MET:HE3	1.47	0.96
1:A:409:GLN:HE22	1:M:2844:VAL:HA	1.35	0.91
1:I:2029:VAL:HG23	1:I:2034:LYS:HG3	1.54	0.89
1:A:506:ALA:O	1:A:507:VAL:HG13	1.76	0.85
1:E:1209:GLN:HE21	1:K:2447:LYS:HD2	1.44	0.83
1:D:1107:VAL:O	1:D:1107:VAL:HG12	1.81	0.81
1:E:1209:GLN:NE2	1:K:2447:LYS:HD2	1.97	0.79
1:H:1847:LYS:HD2	1:K:2409:GLN:HE21	1.50	0.75
1:F:1444:VAL:HA	1:L:2609:GLN:HE22	1.54	0.72
1:G:1707:VAL:O	1:G:1707:VAL:HG12	1.89	0.72
1:C:820:ARG:HD3	1:C:823:MET:CE	2.18	0.71
1:J:2220:ARG:HD3	1:J:2223:MET:CE	2.19	0.71
1:K:2420:ARG:HD3	1:K:2423:MET:CE	2.19	0.71
1:I:2009:GLN:HE21	1:N:3047:LYS:HD2	1.56	0.71
1:M:2820:ARG:HD3	1:M:2823:MET:CE	2.20	0.70
1:I:2020:ARG:HD3	1:I:2023:MET:CE	2.18	0.70
1:B:620:ARG:HD3	1:B:623:MET:CE	2.19	0.69
1:F:1407:GLU:CG	1:F:1456:LYS:HB3	2.22	0.69
1:G:1609:GLN:NE2	1:L:2644:VAL:HA	1.97	0.69
1:A:420:ARG:HD3	1:A:423:MET:CE	2.20	0.69
1:H:1847:LYS:HD2	1:K:2409:GLN:NE2	2.07	0.69
1:E:1307:VAL:O	1:E:1307:VAL:HG23	1.92	0.69
1:G:1620:ARG:HD3	1:G:1623:MET:CE	2.19	0.69
1:L:2620:ARG:HD3	1:L:2623:MET:CE	2.21	0.69
1:E:1220:ARG:HD3	1:E:1223:MET:CE	2.19	0.68
1:K:2506:ALA:O	1:K:2507:VAL:HG13	1.94	0.68
1:I:2009:GLN:HE22	1:N:3044:VAL:HA	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1266:GLU:HG3	1:L:2700:GLY:HA2	1.75	0.67
1:H:1820:ARG:HD3	1:H:1823:MET:CE	2.21	0.67
1:N:3020:ARG:HD3	1:N:3023:MET:CE	2.21	0.67
1:D:1009:GLN:HE22	1:E:1244:VAL:HA	1.59	0.66
1:C:825:THR:HG22	1:C:837:THR:HG22	1.78	0.65
1:I:2009:GLN:NE2	1:N:3047:LYS:HD2	2.13	0.64
1:G:1607:GLU:CG	1:G:1656:LYS:HB3	2.27	0.64
1:G:1664:LEU:O	1:G:1667:VAL:HG22	1.98	0.64
1:M:2864:LEU:O	1:M:2867:VAL:HG22	1.99	0.63
1:E:1226:THR:O	1:E:1229:VAL:HG22	1.98	0.62
1:M:2825:THR:HG22	1:M:2837:THR:HG22	1.82	0.61
1:F:1420:ARG:HD3	1:F:1423:MET:CE	2.22	0.61
1:D:1007:GLU:CG	1:D:1056:LYS:HB3	2.31	0.61
1:C:844:VAL:HA	1:F:1409:GLN:HE22	1.65	0.60
1:J:2207:GLU:CG	1:J:2256:LYS:HB3	2.30	0.60
1:H:1844:VAL:HA	1:K:2409:GLN:HE22	1.67	0.60
1:N:3007:GLU:CG	1:N:3056:LYS:HB3	2.31	0.60
1:G:1625:THR:HG22	1:G:1637:THR:HG22	1.82	0.60
1:B:644:VAL:HA	1:N:3009:GLN:HE22	1.68	0.59
1:N:3025:THR:HG22	1:N:3037:THR:HG22	1.85	0.58
1:F:1407:GLU:HG3	1:F:1456:LYS:HB3	1.85	0.58
1:E:1225:THR:HG22	1:E:1237:THR:HG22	1.84	0.58
1:C:847:LYS:HD2	1:F:1409:GLN:HE21	1.69	0.58
1:F:1408:GLU:O	1:F:1412:ILE:HG12	2.04	0.58
1:A:408:GLU:O	1:A:412:ILE:HG12	2.04	0.58
1:K:2506:ALA:C	1:K:2507:VAL:HG22	2.25	0.58
1:C:808:GLU:O	1:C:812:ILE:HG12	2.04	0.57
1:D:1008:GLU:O	1:D:1012:ILE:HG12	2.04	0.57
1:L:2635:TYR:O	1:L:2639:GLU:HB2	2.04	0.57
1:I:2026:THR:HG23	1:I:2034:LYS:NZ	2.19	0.57
1:D:1020:ARG:HD3	1:D:1023:MET:CE	2.23	0.57
1:L:2608:GLU:O	1:L:2612:ILE:HG12	2.05	0.57
1:M:2807:GLU:CG	1:M:2856:LYS:HB3	2.33	0.57
1:E:1209:GLN:HE22	1:K:2444:VAL:HA	1.70	0.56
1:E:1208:GLU:O	1:E:1212:ILE:HG12	2.04	0.56
1:H:1825:THR:HG22	1:H:1837:THR:HG22	1.87	0.56
1:N:3008:GLU:O	1:N:3012:ILE:HG12	2.05	0.56
1:A:426:THR:HG23	1:A:434:LYS:HE3	1.87	0.56
1:G:1666:GLU:OE1	1:K:2497:ILE:HA	2.04	0.56
1:B:608:GLU:O	1:B:612:ILE:HG12	2.04	0.56
1:L:2607:GLU:CG	1:L:2656:LYS:HB3	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2693:GLU:HG2	1:L:2704:VAL:O	2.05	0.56
1:I:2026:THR:HG23	1:I:2034:LYS:HZ1	1.69	0.56
1:J:2208:GLU:O	1:J:2212:ILE:HG12	2.06	0.56
1:I:2008:GLU:O	1:I:2012:ILE:HG12	2.06	0.56
1:M:2808:GLU:O	1:M:2812:ILE:HG12	2.06	0.56
1:G:1608:GLU:O	1:G:1612:ILE:HG12	2.06	0.55
1:J:2293:GLU:HG2	1:J:2304:VAL:O	2.07	0.55
1:M:2826:THR:HG23	1:M:2834:LYS:NZ	2.22	0.55
1:H:1808:GLU:O	1:H:1812:ILE:HG12	2.07	0.55
1:L:2625:THR:HG22	1:L:2637:THR:HG22	1.87	0.55
1:K:2407:GLU:CG	1:K:2456:LYS:HB3	2.38	0.54
1:I:2026:THR:O	1:I:2029:VAL:HG22	2.07	0.54
1:J:2235:TYR:O	1:J:2239:GLU:HB2	2.06	0.54
1:J:2225:THR:HG22	1:J:2237:THR:HG22	1.89	0.54
1:H:1893:GLU:HG2	1:H:1904:VAL:O	2.08	0.54
1:M:2893:GLU:HG2	1:M:2904:VAL:O	2.08	0.54
1:I:2026:THR:OG1	1:I:2034:LYS:HG2	2.08	0.54
1:M:2825:THR:HG22	1:M:2837:THR:CG2	2.38	0.54
1:A:407:GLU:CG	1:A:456:LYS:HB3	2.39	0.53
1:H:1864:LEU:O	1:H:1867:VAL:HG22	2.08	0.53
1:M:2867:VAL:HG23	1:M:2868:TYR:N	2.24	0.53
1:G:1667:VAL:HG23	1:G:1668:TYR:N	2.23	0.53
1:K:2408:GLU:O	1:K:2412:ILE:HG12	2.08	0.53
1:I:2007:GLU:CG	1:I:2056:LYS:HB3	2.38	0.53
1:A:493:GLU:HG2	1:A:504:VAL:O	2.09	0.53
1:K:2506:ALA:O	1:K:2507:VAL:HG22	2.08	0.53
1:C:825:THR:HG22	1:C:837:THR:CG2	2.39	0.53
1:I:2029:VAL:CG2	1:I:2034:LYS:HG3	2.35	0.52
1:F:1493:GLU:HG2	1:F:1504:VAL:O	2.09	0.52
1:I:2097:ILE:HA	1:M:2866:GLU:OE1	2.09	0.52
1:M:2907:VAL:HG12	1:M:2907:VAL:O	2.08	0.52
1:G:1607:GLU:HG3	1:G:1656:LYS:HB3	1.91	0.52
1:K:2493:GLU:HG2	1:K:2504:VAL:O	2.09	0.52
1:L:2625:THR:HG22	1:L:2637:THR:CG2	2.40	0.52
1:B:693:GLU:HG2	1:B:704:VAL:O	2.10	0.52
1:G:1693:GLU:HG2	1:G:1704:VAL:O	2.09	0.52
1:N:3093:GLU:HG2	1:N:3104:VAL:O	2.10	0.52
1:D:1025:THR:HG22	1:D:1037:THR:HG22	1.92	0.52
1:G:1666:GLU:HG3	1:K:2500:GLY:HA2	1.91	0.52
1:J:2207:GLU:HG2	1:J:2256:LYS:HB3	1.92	0.51
1:D:1009:GLN:HE21	1:E:1247:LYS:HD2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1293:GLU:HG2	1:E:1304:VAL:O	2.10	0.51
1:H:1807:GLU:CG	1:H:1856:LYS:HB3	2.40	0.51
1:F:1419:PHE:CE2	1:F:1423:MET:HE1	2.46	0.51
1:H:1867:VAL:HG23	1:H:1868:TYR:N	2.26	0.51
1:A:425:THR:HG22	1:A:437:THR:HG22	1.93	0.51
1:C:826:THR:O	1:C:829:VAL:HG22	2.10	0.50
1:F:1467:VAL:HG12	1:F:1494:ALA:HB1	1.93	0.50
1:M:2826:THR:HG23	1:M:2834:LYS:HZ2	1.75	0.50
1:A:506:ALA:C	1:A:507:VAL:HG22	2.32	0.50
1:D:1107:VAL:O	1:D:1107:VAL:CG1	2.53	0.50
1:C:893:GLU:HG2	1:C:904:VAL:O	2.12	0.50
1:D:1093:GLU:HG2	1:D:1104:VAL:O	2.12	0.50
1:M:2842:PHE:CZ	1:M:2868:TYR:HE1	2.29	0.50
1:B:644:VAL:HG21	1:F:1428:ASN:OD1	2.11	0.50
1:L:2607:GLU:HG2	1:L:2656:LYS:HB3	1.94	0.50
1:H:1825:THR:HG22	1:H:1837:THR:CG2	2.43	0.49
1:C:847:LYS:HD2	1:F:1409:GLN:NE2	2.26	0.49
1:I:2093:GLU:HG2	1:I:2104:VAL:O	2.13	0.49
1:C:807:GLU:CG	1:C:856:LYS:HB3	2.42	0.49
1:G:1664:LEU:O	1:G:1667:VAL:CG2	2.60	0.49
1:N:3025:THR:HG22	1:N:3037:THR:CG2	2.41	0.49
1:G:1625:THR:HG22	1:G:1637:THR:CG2	2.42	0.49
1:D:1007:GLU:HG3	1:D:1056:LYS:HB3	1.95	0.49
1:J:2225:THR:HG22	1:J:2237:THR:CG2	2.43	0.49
1:N:3007:GLU:HG2	1:N:3056:LYS:HB3	1.96	0.48
1:D:1007:GLU:HA	1:D:1007:GLU:OE1	2.14	0.47
1:N:3007:GLU:HG3	1:N:3056:LYS:HB3	1.94	0.47
1:D:1019:PHE:CE2	1:D:1023:MET:HE1	2.50	0.47
1:E:1225:THR:HG22	1:E:1237:THR:CG2	2.43	0.47
1:L:2664:LEU:O	1:L:2667:VAL:HG22	2.14	0.47
1:N:3007:GLU:OE1	1:N:3007:GLU:HA	2.15	0.47
1:L:2657:ALA:C	1:L:2659:GLN:OE1	2.54	0.47
1:L:2667:VAL:HG23	1:L:2668:TYR:N	2.29	0.47
1:B:607:GLU:CG	1:B:656:LYS:HB3	2.45	0.46
1:B:607:GLU:OE1	1:B:607:GLU:HA	2.15	0.46
1:F:1407:GLU:HA	1:F:1407:GLU:OE1	2.15	0.46
1:F:1464:LEU:O	1:F:1467:VAL:HG22	2.15	0.46
1:H:1807:GLU:HA	1:H:1807:GLU:OE1	2.15	0.46
1:J:2207:GLU:OE1	1:J:2207:GLU:HA	2.15	0.46
1:D:1009:GLN:NE2	1:E:1247:LYS:HD2	2.30	0.46
1:L:2659:GLN:OE1	1:L:2659:GLN:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2807:GLU:HG3	1:M:2856:LYS:HB3	1.97	0.46
1:G:1666:GLU:CG	1:K:2500:GLY:HA2	2.46	0.46
1:E:1219:PHE:CE2	1:E:1223:MET:HE1	2.51	0.46
1:M:2858:PRO:HB3	1:N:3058:PRO:HB3	1.98	0.46
1:M:2858:PRO:CB	1:N:3058:PRO:HB3	2.46	0.46
1:F:1407:GLU:HG2	1:F:1456:LYS:HB3	1.95	0.45
1:M:2807:GLU:OE1	1:M:2807:GLU:HA	2.16	0.45
1:M:2904:VAL:HG23	1:M:2904:VAL:O	2.16	0.45
1:F:1425:THR:HG22	1:F:1437:THR:HG22	1.98	0.45
1:G:1629:VAL:HG21	1:G:1634:LYS:HA	1.97	0.45
1:H:1857:ALA:C	1:H:1859:GLN:OE1	2.55	0.45
1:I:2100:GLY:HA2	1:M:2866:GLU:HG3	1.99	0.45
1:N:3057:ALA:C	1:N:3059:GLN:OE1	2.55	0.45
1:I:2064:LEU:O	1:I:2067:VAL:HG22	2.16	0.45
1:H:1807:GLU:HG3	1:H:1856:LYS:HB3	1.99	0.45
1:A:407:GLU:HA	1:A:407:GLU:OE1	2.17	0.45
1:B:629:VAL:HG23	1:B:633:ASP:HB2	1.98	0.45
1:F:1467:VAL:HG23	1:F:1468:TYR:N	2.32	0.45
1:I:2057:ALA:C	1:I:2059:GLN:OE1	2.56	0.45
1:D:1029:VAL:HG21	1:D:1034:LYS:HA	1.99	0.44
1:J:2267:VAL:CG2	1:J:2268:TYR:N	2.79	0.44
1:B:625:THR:HG22	1:B:637:THR:HG22	1.99	0.44
1:H:1907:VAL:O	1:H:1907:VAL:HG12	2.16	0.44
1:J:2257:ALA:C	1:J:2259:GLN:OE1	2.56	0.44
1:J:2207:GLU:HG3	1:J:2256:LYS:HB3	1.98	0.44
1:H:1859:GLN:N	1:H:1859:GLN:OE1	2.51	0.44
1:K:2457:ALA:C	1:K:2459:GLN:OE1	2.55	0.44
1:L:2625:THR:CG2	1:L:2637:THR:HG22	2.48	0.44
1:G:1607:GLU:HG2	1:G:1656:LYS:HB3	1.98	0.44
1:I:2007:GLU:HA	1:I:2007:GLU:OE1	2.18	0.44
1:A:504:VAL:HG23	1:A:504:VAL:O	2.18	0.44
1:M:2858:PRO:HB3	1:N:3058:PRO:CB	2.48	0.44
1:M:2831:PRO:HA	1:M:2834:LYS:HD2	1.98	0.44
1:G:1607:GLU:HA	1:G:1607:GLU:OE1	2.18	0.44
1:L:2607:GLU:HA	1:L:2607:GLU:OE1	2.17	0.44
1:E:1257:ALA:C	1:E:1259:GLN:OE1	2.56	0.43
1:E:1207:GLU:OE1	1:E:1207:GLU:HA	2.18	0.43
1:F:1429:VAL:HG21	1:F:1434:LYS:HA	2.00	0.43
1:D:1026:THR:HG23	1:D:1034:LYS:HE3	2.00	0.43
1:F:1459:GLN:OE1	1:F:1459:GLN:N	2.51	0.43
1:M:2829:VAL:HG21	1:M:2834:LYS:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:857:ALA:C	1:C:859:GLN:OE1	2.56	0.43
1:D:1066:GLU:HG3	1:F:1500:GLY:HA2	2.00	0.43
1:G:1704:VAL:O	1:G:1704:VAL:HG23	2.18	0.43
1:K:2407:GLU:HA	1:K:2407:GLU:OE1	2.19	0.43
1:C:807:GLU:HA	1:C:807:GLU:OE1	2.19	0.43
1:N:3031:PRO:O	1:N:3034:LYS:HB2	2.18	0.43
1:A:420:ARG:HA	1:A:423:MET:HE3	2.01	0.43
1:K:2407:GLU:HG3	1:K:2456:LYS:HB3	2.01	0.43
1:N:3025:THR:CG2	1:N:3037:THR:HG22	2.48	0.43
1:K:2464:LEU:HD12	1:K:2464:LEU:HA	1.85	0.43
1:B:619:PHE:CE2	1:B:623:MET:HE1	2.54	0.42
1:J:2259:GLN:N	1:J:2259:GLN:OE1	2.51	0.42
1:E:1266:GLU:OE1	1:L:2697:ILE:HA	2.18	0.42
1:J:2208:GLU:HG3	1:J:2260:LEU:HD22	2.01	0.42
1:M:2859:GLN:OE1	1:M:2859:GLN:N	2.51	0.42
1:I:2066:GLU:OE1	1:M:2897:ILE:HA	2.19	0.42
1:E:1250:LEU:O	1:E:1254:VAL:HG23	2.19	0.42
1:E:1304:VAL:HG23	1:E:1304:VAL:O	2.19	0.42
1:I:2059:GLN:N	1:I:2059:GLN:OE1	2.51	0.42
1:L:2704:VAL:O	1:L:2704:VAL:HG23	2.19	0.42
1:J:2264:LEU:HA	1:J:2264:LEU:HD12	1.89	0.42
1:A:504:VAL:HG13	1:N:3070:ALA:HA	2.00	0.42
1:A:470:ALA:HA	1:N:3104:VAL:HG13	2.00	0.42
1:B:657:ALA:C	1:B:659:GLN:OE1	2.58	0.42
1:D:1100:GLY:HA2	1:F:1466:GLU:HG3	2.02	0.42
1:J:2267:VAL:O	1:J:2268:TYR:C	2.57	0.42
1:N:3026:THR:O	1:N:3029:VAL:HG22	2.20	0.42
1:A:459:GLN:HA	1:B:654:VAL:HG11	2.01	0.42
1:D:1104:VAL:HG13	1:F:1470:ALA:HA	2.02	0.42
1:F:1504:VAL:O	1:F:1504:VAL:HG23	2.19	0.42
1:G:1636:LYS:HG2	1:G:1636:LYS:H	1.36	0.42
1:G:1659:GLN:N	1:G:1659:GLN:OE1	2.52	0.42
1:I:2058:PRO:HB3	1:J:2258:PRO:HB3	2.02	0.41
1:B:626:THR:HG23	1:B:634:LYS:HE3	2.02	0.41
1:K:2407:GLU:HG2	1:K:2456:LYS:HB3	2.03	0.41
1:A:409:GLN:NE2	1:M:2844:VAL:HA	2.18	0.41
1:N:3059:GLN:OE1	1:N:3059:GLN:N	2.51	0.41
1:G:1658:PRO:HB3	1:H:1858:PRO:HB3	2.01	0.41
1:G:1664:LEU:HA	1:G:1664:LEU:HD12	1.86	0.41
1:E:1207:GLU:CG	1:E:1256:LYS:HB3	2.50	0.41
1:J:2247:LYS:HD2	1:M:2809:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1697:ILE:HA	1:K:2466:GLU:OE1	2.20	0.41
1:G:1704:VAL:HG13	1:K:2470:ALA:HA	2.01	0.41
1:L:2608:GLU:HG3	1:L:2660:LEU:HD22	2.03	0.41
1:H:1867:VAL:CG2	1:H:1868:TYR:N	2.82	0.41
1:I:2020:ARG:HA	1:I:2023:MET:HE3	2.03	0.41
1:M:2857:ALA:C	1:M:2859:GLN:OE1	2.59	0.41
1:D:1059:GLN:OE1	1:D:1059:GLN:N	2.51	0.41
1:F:1457:ALA:C	1:F:1459:GLN:OE1	2.58	0.41
1:G:1642:PHE:CZ	1:G:1668:TYR:HE2	2.39	0.41
1:F:1464:LEU:HD12	1:F:1464:LEU:HA	1.86	0.41
1:H:1868:TYR:CD2	1:H:1891:PHE:HE1	2.39	0.41
1:B:688:VAL:O	1:B:692:SER:HB2	2.21	0.41
1:D:1057:ALA:C	1:D:1059:GLN:OE1	2.58	0.41
1:E:1229:VAL:HG23	1:E:1234:LYS:HG2	2.03	0.41
1:M:2807:GLU:HG2	1:M:2856:LYS:HB3	1.99	0.41
1:A:457:ALA:C	1:A:459:GLN:OE1	2.59	0.41
1:A:454:VAL:HG11	1:B:659:GLN:HA	2.02	0.41
1:D:1029:VAL:HG23	1:D:1034:LYS:HG3	2.02	0.41
1:A:459:GLN:OE1	1:A:459:GLN:N	2.54	0.40
1:G:1658:PRO:CB	1:H:1858:PRO:HB3	2.51	0.40
1:G:1657:ALA:C	1:G:1659:GLN:OE1	2.59	0.40
1:J:2304:VAL:O	1:J:2304:VAL:HG23	2.19	0.40
1:K:2458:PRO:HB3	1:L:2658:PRO:HB3	2.02	0.40
1:A:407:GLU:HG3	1:A:456:LYS:HB3	2.03	0.40
1:C:850:LEU:O	1:C:854:VAL:HG23	2.21	0.40
1:H:1825:THR:CG2	1:H:1837:THR:HG22	2.51	0.40
1:A:425:THR:HG22	1:A:437:THR:CG2	2.51	0.40
1:B:664:LEU:HD12	1:B:664:LEU:HA	1.88	0.40
1:C:859:GLN:N	1:C:859:GLN:OE1	2.54	0.40
1:C:904:VAL:O	1:C:904:VAL:HG23	2.20	0.40
1:D:1067:VAL:HG23	1:D:1094:ALA:HB3	2.03	0.40
1:H:1820:ARG:HA	1:H:1823:MET:HE3	2.02	0.40
1:I:2007:GLU:HG3	1:I:2056:LYS:HB3	2.03	0.40
1:K:2429:VAL:HG23	1:K:2434:LYS:CG	2.51	0.40
1:M:2864:LEU:HA	1:M:2864:LEU:HD12	1.85	0.40
1:A:506:ALA:O	1:A:507:VAL:HG22	2.22	0.40
1:B:636:LYS:HE3	1:F:1436:LYS:NZ	2.37	0.40
1:H:1864:LEU:HD12	1:H:1864:LEU:HA	1.81	0.40
1:H:1904:VAL:HG23	1:H:1904:VAL:O	2.21	0.40
1:L:2661:VAL:N	1:L:2662:PRO:HD2	2.36	0.40
1:M:2829:VAL:CG2	1:M:2834:LYS:HA	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1836:LYS:HG3	1:H:1837:THR:N	2.36	0.40
1:I:2025:THR:HG22	1:I:2037:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/111 (92%)	97 (95%)	5 (5%)	0	100	100
1	B	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
1	C	102/111 (92%)	96 (94%)	5 (5%)	1 (1%)	15	44
1	D	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
1	E	102/111 (92%)	97 (95%)	5 (5%)	0	100	100
1	F	102/111 (92%)	97 (95%)	4 (4%)	1 (1%)	15	44
1	G	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
1	H	102/111 (92%)	96 (94%)	5 (5%)	1 (1%)	15	44
1	I	102/111 (92%)	97 (95%)	5 (5%)	0	100	100
1	J	102/111 (92%)	97 (95%)	5 (5%)	0	100	100
1	K	102/111 (92%)	97 (95%)	4 (4%)	1 (1%)	15	44
1	L	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
1	M	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
1	N	102/111 (92%)	95 (93%)	5 (5%)	2 (2%)	7	24
All	All	1428/1554 (92%)	1355 (95%)	67 (5%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	3027	ALA
1	C	831	PRO
1	K	2431	PRO
1	F	1431	PRO
1	N	3031	PRO
1	H	1831	PRO

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	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	B	81/85 (95%)	76 (94%)	5 (6%)	18 47
1	C	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	D	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	E	81/85 (95%)	74 (91%)	7 (9%)	10 30
1	F	81/85 (95%)	77 (95%)	4 (5%)	25 57
1	G	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	H	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	I	81/85 (95%)	77 (95%)	4 (5%)	25 57
1	J	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	K	81/85 (95%)	75 (93%)	6 (7%)	13 37
1	L	81/85 (95%)	77 (95%)	4 (5%)	25 57
1	M	81/85 (95%)	76 (94%)	5 (6%)	18 47
1	N	81/85 (95%)	76 (94%)	5 (6%)	18 47
All	All	1134/1190 (95%)	1058 (93%)	76 (7%)	16 43

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	THR
1	A	439	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	GLN
1	A	464	LEU
1	A	467	VAL
1	A	507	VAL
1	B	626	THR
1	B	639	GLU
1	B	659	GLN
1	B	664	LEU
1	B	692	SER
1	C	826	THR
1	C	839	GLU
1	C	859	GLN
1	C	864	LEU
1	C	867	VAL
1	C	898	ILE
1	D	1026	THR
1	D	1039	GLU
1	D	1059	GLN
1	D	1064	LEU
1	D	1066	GLU
1	D	1067	VAL
1	E	1226	THR
1	E	1239	GLU
1	E	1259	GLN
1	E	1264	LEU
1	E	1266	GLU
1	E	1267	VAL
1	E	1307	VAL
1	F	1426	THR
1	F	1439	GLU
1	F	1459	GLN
1	F	1464	LEU
1	G	1626	THR
1	G	1636	LYS
1	G	1639	GLU
1	G	1659	GLN
1	G	1664	LEU
1	G	1666	GLU
1	H	1826	THR
1	H	1839	GLU
1	H	1859	GLN
1	H	1864	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1865	ASP
1	H	1898	ILE
1	I	2026	THR
1	I	2039	GLU
1	I	2059	GLN
1	I	2064	LEU
1	J	2226	THR
1	J	2236	LYS
1	J	2239	GLU
1	J	2259	GLN
1	J	2264	LEU
1	J	2267	VAL
1	K	2426	THR
1	K	2431	PRO
1	K	2439	GLU
1	K	2459	GLN
1	K	2464	LEU
1	K	2507	VAL
1	L	2626	THR
1	L	2639	GLU
1	L	2659	GLN
1	L	2664	LEU
1	M	2826	THR
1	M	2829	VAL
1	M	2839	GLU
1	M	2859	GLN
1	M	2864	LEU
1	N	3026	THR
1	N	3039	GLU
1	N	3059	GLN
1	N	3064	LEU
1	N	3098	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	C	828	ASN
1	C	849	ASN
1	D	1009	GLN
1	E	1209	GLN
1	E	1228	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1249	ASN
1	F	1409	GLN
1	G	1609	GLN
1	G	1628	ASN
1	H	1849	ASN
1	I	2009	GLN
1	I	2028	ASN
1	I	2049	ASN
1	J	2249	ASN
1	K	2409	GLN
1	K	2428	ASN
1	K	2449	ASN
1	L	2649	ASN
1	M	2809	GLN
1	M	2828	ASN
1	N	3049	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 35 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	104/111 (93%)	0.02	1 (0%) 82 77	16, 35, 70, 86	0
1	B	104/111 (93%)	-0.00	1 (0%) 82 77	17, 34, 72, 101	0
1	C	104/111 (93%)	-0.04	0 100 100	14, 32, 73, 83	0
1	D	104/111 (93%)	-0.11	0 100 100	11, 30, 71, 88	0
1	E	104/111 (93%)	-0.05	0 100 100	12, 33, 64, 78	0
1	F	104/111 (93%)	-0.14	0 100 100	15, 31, 70, 81	0
1	G	104/111 (93%)	-0.01	0 100 100	12, 34, 67, 84	0
1	H	104/111 (93%)	0.05	2 (1%) 66 59	15, 40, 84, 95	0
1	I	104/111 (93%)	0.02	0 100 100	11, 36, 74, 101	0
1	J	104/111 (93%)	-0.02	1 (0%) 82 77	10, 33, 72, 99	0
1	K	104/111 (93%)	-0.02	2 (1%) 66 59	11, 36, 75, 102	0
1	L	104/111 (93%)	-0.01	3 (2%) 51 41	13, 33, 75, 101	0
1	M	104/111 (93%)	-0.07	0 100 100	9, 32, 68, 85	0
1	N	104/111 (93%)	0.05	2 (1%) 66 59	13, 40, 82, 108	0
All	All	1456/1554 (93%)	-0.02	12 (0%) 86 81	9, 35, 75, 108	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2428	ASN	3.8
1	A	507	VAL	3.1
1	N	3005	THR	3.0
1	L	2605	THR	2.9
1	K	2507	VAL	2.7
1	H	1827	ALA	2.7
1	J	2205	THR	2.6
1	B	605	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	1828	ASN	2.3
1	L	2628	ASN	2.2
1	N	3004	ALA	2.2
1	L	2604	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ARS	B	7002	1/1	0.91	0.12	68,68,68,68	0
3	ARS	I	7009	1/1	0.92	0.16	56,56,56,56	0
2	ZN	M	6013	1/1	0.94	0.15	32,32,32,32	0
3	ARS	D	7004	1/1	0.94	0.10	66,66,66,66	0
3	ARS	K	7007	1/1	0.95	0.15	63,63,63,63	0
3	ARS	C	7003	1/1	0.96	0.12	60,60,60,60	0
2	ZN	E	6005	1/1	0.97	0.14	25,25,25,25	0
3	ARS	N	7001	1/1	0.97	0.10	61,61,61,61	0
2	ZN	K	5011	1/1	0.97	0.17	28,28,28,28	0
2	ZN	A	5001	1/1	0.97	0.17	29,29,29,29	0
2	ZN	C	6003	1/1	0.97	0.13	27,27,27,27	0
2	ZN	A	6001	1/1	0.97	0.12	28,28,28,28	0
2	ZN	E	5005	1/1	0.97	0.12	30,30,30,30	0
3	ARS	L	7005	1/1	0.97	0.13	57,57,57,57	0
2	ZN	J	6010	1/1	0.98	0.12	30,30,30,30	0
2	ZN	K	6011	1/1	0.98	0.12	28,28,28,28	0
2	ZN	G	6007	1/1	0.98	0.12	24,24,24,24	0
2	ZN	L	5012	1/1	0.98	0.13	19,19,19,19	0
2	ZN	H	6008	1/1	0.98	0.13	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	G	5007	1/1	0.98	0.14	25,25,25,25	0
2	ZN	I	5009	1/1	0.98	0.16	23,23,23,23	0
2	ZN	M	5013	1/1	0.98	0.13	28,28,28,28	0
2	ZN	I	6009	1/1	0.98	0.17	25,25,25,25	0
2	ZN	L	6012	1/1	0.98	0.13	26,26,26,26	0
2	ZN	H	5008	1/1	0.98	0.13	29,29,29,29	0
2	ZN	F	5006	1/1	0.99	0.15	23,23,23,23	0
2	ZN	D	5004	1/1	0.99	0.12	25,25,25,25	0
2	ZN	D	6004	1/1	0.99	0.13	28,28,28,28	0
2	ZN	B	6002	1/1	0.99	0.12	29,29,29,29	0
2	ZN	J	5010	1/1	0.99	0.13	22,22,22,22	0
2	ZN	F	6006	1/1	0.99	0.14	26,26,26,26	0
2	ZN	C	5003	1/1	0.99	0.15	32,32,32,32	0
2	ZN	N	6014	1/1	0.99	0.16	26,26,26,26	0
2	ZN	N	5014	1/1	0.99	0.09	27,27,27,27	0
2	ZN	B	5002	1/1	0.99	0.13	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.