



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:32 AM UTC

PDB ID : 3EZJ / pdb_00003ezj
Title : Crystal structure of the N-terminal domain of the secretin GspD from ETEC determined with the assistance of a nanobody
Authors : Korotkov, K.V.; Pardon, E.; Steyaert, J.; Hol, W.G.
Deposited on : 2008-10-22
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

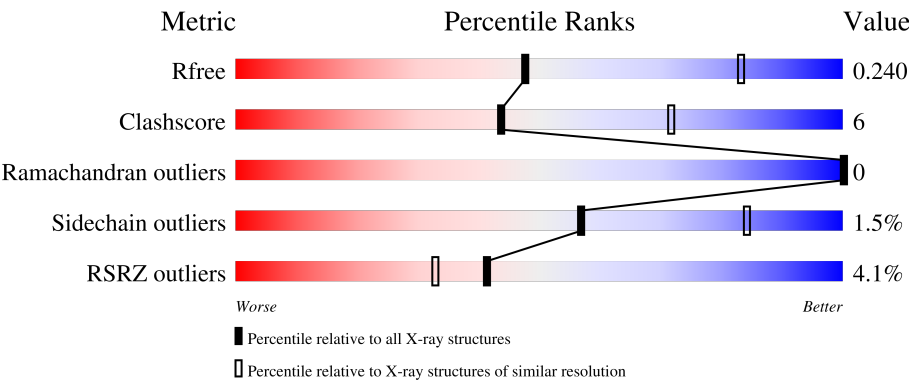
1 Overall quality at a glance i

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	241	3% 69% 12% 18%
1	C	241	4% 71% 11% 18%
1	E	241	6% 67% 15% 18%
1	G	241	7% 72% 10% 17%
2	B	126	% 80% 15% 5%

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Mol	Chain	Length	Quality of chain		
2	D	126		84%	11% 5%
2	F	126		87%	8% 5%
2	H	126		83%	13% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	D	127	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10048 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 General secretion pathway protein GspD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1535	954	275	299	7			
1	C	197	Total	C	N	O	S	0	0	0
			1525	948	273	297	7			
1	E	197	Total	C	N	O	S	0	0	0
			1524	947	273	297	7			
1	G	199	Total	C	N	O	S	0	0	0
			1540	957	276	300	7			

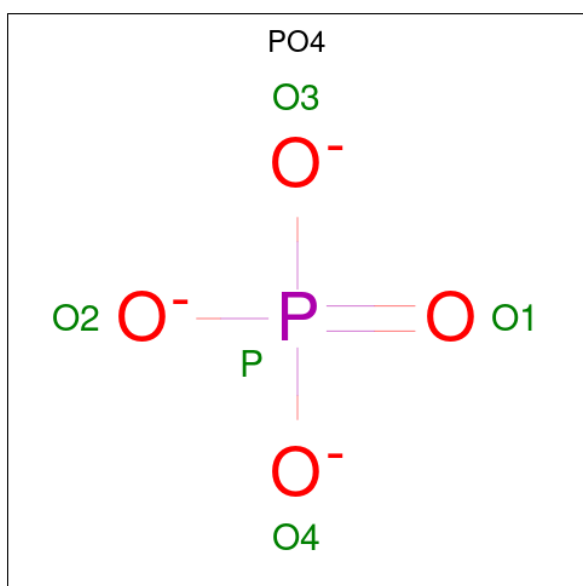
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP B3IFK0
A	-2	ALA	-	expression tag	UNP B3IFK0
A	-1	MET	-	expression tag	UNP B3IFK0
A	38	ALA	LYS	engineered mutation	UNP B3IFK0
C	-3	GLY	-	expression tag	UNP B3IFK0
C	-2	ALA	-	expression tag	UNP B3IFK0
C	-1	MET	-	expression tag	UNP B3IFK0
C	38	ALA	LYS	engineered mutation	UNP B3IFK0
E	-3	GLY	-	expression tag	UNP B3IFK0
E	-2	ALA	-	expression tag	UNP B3IFK0
E	-1	MET	-	expression tag	UNP B3IFK0
E	38	ALA	LYS	engineered mutation	UNP B3IFK0
G	-3	GLY	-	expression tag	UNP B3IFK0
G	-2	ALA	-	expression tag	UNP B3IFK0
G	-1	MET	-	expression tag	UNP B3IFK0
G	38	ALA	LYS	engineered mutation	UNP B3IFK0

- Molecule 2 is a protein called NANOBODY NBGSPD_7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			904	554	162	183	5			
2	D	120	Total	C	N	O	S	0	0	0
			904	554	162	183	5			
2	F	120	Total	C	N	O	S	0	0	0
			904	554	162	183	5			
2	H	120	Total	C	N	O	S	0	0	0
			904	554	162	183	5			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0

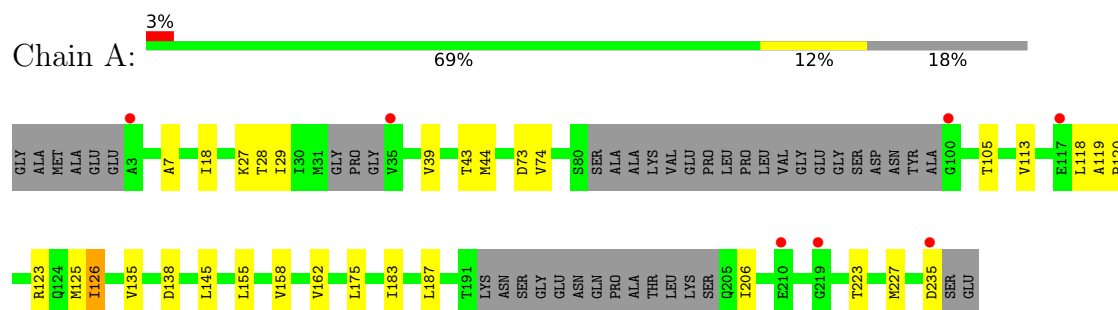
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	C	32	Total 32	O 32	0	0
5	E	30	Total 30	O 30	0	0
5	G	29	Total 29	O 29	0	0
5	B	32	Total 32	O 32	0	0
5	D	43	Total 43	O 43	0	0
5	F	38	Total 38	O 38	0	0
5	H	35	Total 35	O 35	0	0

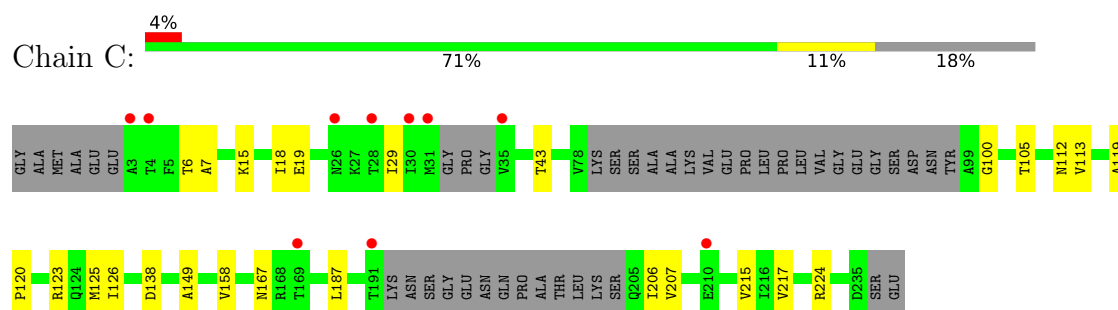
3 Residue-property plots [i](#)

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

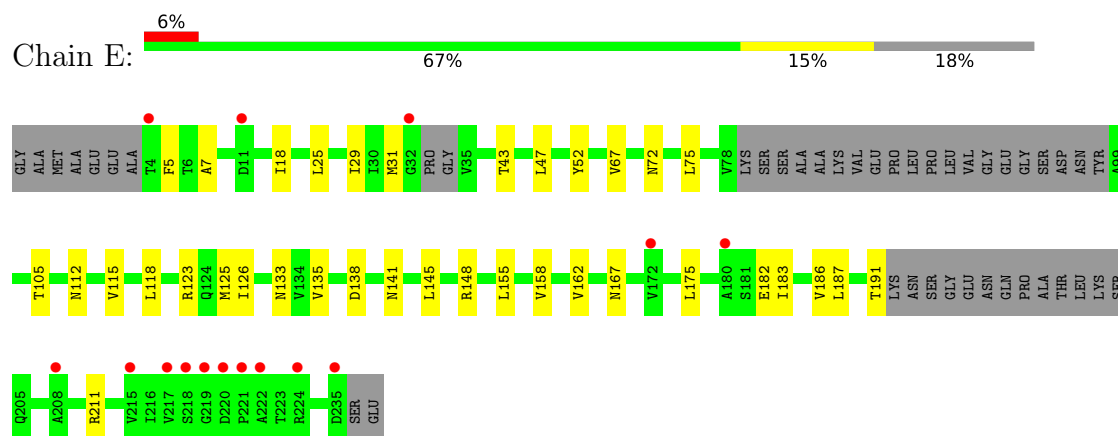
- Molecule 1: General secretion pathway protein GspD



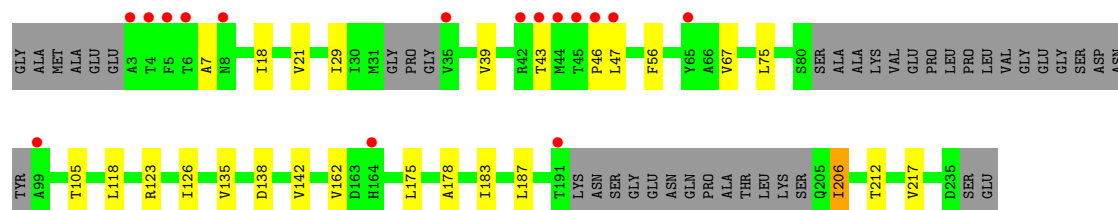
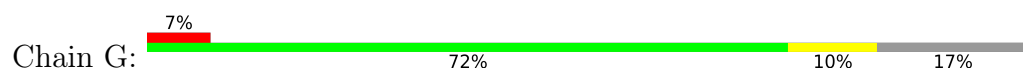
- Molecule 1: General secretion pathway protein GspD



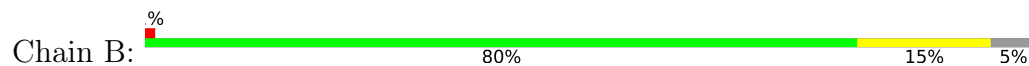
- Molecule 1: General secretion pathway protein GspD



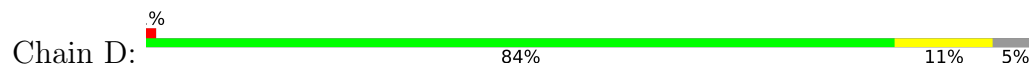
- Molecule 1: General secretion pathway protein GspD



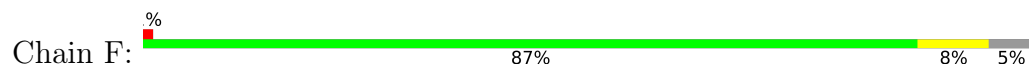
• Molecule 2: NANOBODY NBGSPD_7



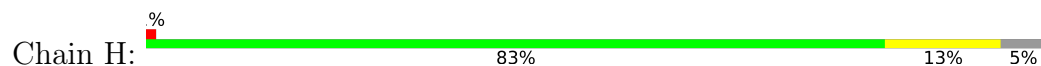
• Molecule 2: NANOBODY NBGSPD_7



• Molecule 2: NANOBODY NBGSPD_7



• Molecule 2: NANOBODY NBGSPD_7



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.52Å 98.52Å 402.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 2.80 47.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.67-2.80) 97.0 (47.67-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.239 0.197 , 0.240	Depositor DCC
R_{free} test set	4372 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10048	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: CL, PO4

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	0/1547	0.73	0/2093
1	C	0.57	0/1537	0.74	0/2081
1	E	0.54	0/1536	0.74	0/2079
1	G	0.56	0/1552	0.72	0/2100
2	B	0.59	0/918	0.71	0/1242
2	D	0.59	0/918	0.75	0/1242
2	F	0.59	0/918	0.74	0/1242
2	H	0.63	0/918	0.75	0/1242
All	All	0.57	0/9844	0.73	0/13321

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	1535	0	1575	20	0
1	C	1525	0	1562	17	0
1	E	1524	0	1560	29	0
1	G	1540	0	1580	25	0
2	B	904	0	874	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	904	0	874	10	0
2	F	904	0	874	8	0
2	H	904	0	874	11	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	2	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	A	25	0	0	1	0
5	B	32	0	0	0	0
5	C	32	0	0	1	0
5	D	43	0	0	0	0
5	E	30	0	0	0	0
5	F	38	0	0	0	0
5	G	29	0	0	0	0
5	H	35	0	0	0	0
All	All	10048	0	9773	120	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 6.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD12	2:B:110:TRP:HA	1.51	0.92
1:E:126:ILE:HD11	1:E:135:VAL:HG23	1.55	0.89
1:C:125:MET:HE3	1:C:158:VAL:HG21	1.62	0.82
1:E:125:MET:HE3	1:E:158:VAL:HG21	1.60	0.82
1:E:175:LEU:HD13	1:E:183:ILE:HD12	1.67	0.77
1:C:18:ILE:CG2	1:C:29:ILE:HG21	2.16	0.75
2:B:20:LEU:HG	2:B:82:MET:HE2	1.67	0.74
2:H:75:LYS:O	2:H:77:THR:HG23	1.89	0.72
1:G:18:ILE:CG2	1:G:29:ILE:HG21	2.20	0.71
1:E:7:ALA:HB3	1:E:43:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG22	1:A:227:MET:HE2	1.78	0.66
1:C:123:ARG:NH1	2:D:37:ASP:OD2	2.31	0.64
1:C:7:ALA:HB3	1:C:43:THR:HG23	1.79	0.64
1:E:18:ILE:CG2	1:E:29:ILE:HG21	2.27	0.64
1:G:175:LEU:HD13	1:G:183:ILE:HD12	1.79	0.63
1:G:18:ILE:HG22	1:G:29:ILE:HG21	1.81	0.62
1:C:207:VAL:HG21	5:C:250:HOH:O	1.99	0.61
1:C:18:ILE:HG22	1:C:29:ILE:HG21	1.82	0.61
1:E:118:LEU:HD21	1:E:162:VAL:HG11	1.82	0.61
2:B:75:LYS:O	2:B:77:THR:HG23	2.01	0.60
1:E:123:ARG:NH1	2:F:37:ASP:OD2	2.33	0.60
1:E:175:LEU:CD1	1:E:183:ILE:HD12	2.32	0.60
1:E:187:LEU:O	1:E:191:THR:HG22	2.01	0.60
1:A:43:THR:HG22	1:A:105:THR:CG2	2.33	0.59
1:E:125:MET:CE	1:E:158:VAL:HG21	2.32	0.59
1:G:175:LEU:CD1	1:G:183:ILE:HD12	2.33	0.59
1:E:18:ILE:HG21	1:E:29:ILE:HG21	1.84	0.59
2:H:20:LEU:HG	2:H:82:MET:HE2	1.84	0.58
2:H:4:LEU:HD12	2:H:110:TRP:HA	1.84	0.58
1:G:43:THR:HA	1:G:105:THR:HG22	1.85	0.58
2:B:82:MET:HE1	2:B:116:VAL:HG21	1.86	0.58
1:G:21:VAL:HG11	1:G:56:PHE:CG	2.40	0.56
2:B:23:ALA:HA	2:B:77:THR:HG22	1.88	0.56
1:A:27:LYS:NZ	1:A:73:ASP:OD1	2.33	0.56
1:E:5:PHE:N	1:E:47:LEU:O	2.39	0.54
2:D:18:LEU:HB2	2:D:82:MET:HE3	1.89	0.54
1:G:178:ALA:CB	1:G:183:ILE:HD11	2.37	0.54
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.89	0.53
1:G:7:ALA:HB3	1:G:43:THR:HG23	1.89	0.53
1:E:118:LEU:CD2	1:E:162:VAL:HG11	2.38	0.53
1:E:125:MET:HG2	1:E:155:LEU:HD23	1.91	0.53
2:F:61:ASP:OD1	3:F:127:PO4:O1	2.27	0.52
1:A:28:THR:HB	1:A:74:VAL:HG22	1.91	0.52
1:A:119:ALA:HB3	1:A:120:PRO:HD3	1.92	0.52
1:A:18:ILE:HG22	1:A:29:ILE:HG21	1.92	0.52
1:A:175:LEU:HD13	1:A:183:ILE:HD12	1.92	0.52
1:A:126:ILE:HD11	1:A:135:VAL:HG23	1.92	0.51
1:C:206:ILE:HG23	1:C:215:VAL:CG1	2.39	0.51
1:C:15:LYS:O	1:C:19:GLU:HG2	2.10	0.51
1:G:118:LEU:HD21	1:G:162:VAL:HG11	1.92	0.51
1:A:138:ASP:HB2	2:B:105:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ILE:HD11	1:G:135:VAL:HG23	1.93	0.50
2:F:20:LEU:HG	2:F:82:MET:HE2	1.92	0.50
1:E:112:ASN:ND2	1:E:167:ASN:HB2	2.27	0.50
2:F:82:MET:HE1	2:F:116:VAL:HG21	1.93	0.50
2:B:51:ILE:HD13	2:B:71:ARG:HB2	1.92	0.50
2:D:20:LEU:HG	2:D:82:MET:HE2	1.92	0.50
1:G:187:LEU:CB	1:G:206:ILE:HD12	2.42	0.49
1:E:138:ASP:HB2	2:F:105:MET:CE	2.42	0.49
1:C:43:THR:HA	1:C:105:THR:HG22	1.94	0.48
1:A:44:MET:HE1	5:A:260:HOH:O	2.13	0.48
2:F:28:ILE:HA	2:F:31:ILE:HD12	1.94	0.48
1:G:21:VAL:HG11	1:G:56:PHE:CD1	2.49	0.48
1:G:138:ASP:HB2	2:H:105:MET:HE3	1.96	0.47
1:C:100:GLY:HA2	1:C:149:ALA:HB3	1.96	0.47
2:H:90:THR:O	2:H:91:ALA:HB2	2.15	0.47
1:A:123:ARG:NH1	2:B:37:ASP:OD2	2.48	0.47
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.97	0.47
1:A:125:MET:HE3	1:A:158:VAL:HG21	1.96	0.47
1:C:119:ALA:HB3	1:C:120:PRO:HD3	1.96	0.47
1:A:7:ALA:HB3	1:A:43:THR:HG23	1.98	0.46
1:A:18:ILE:CG2	1:A:29:ILE:HG21	2.46	0.45
1:A:118:LEU:HD21	1:A:162:VAL:HB	1.98	0.45
1:E:138:ASP:HB2	2:F:105:MET:HE3	1.98	0.45
1:A:125:MET:HG2	1:A:155:LEU:HD23	1.98	0.45
1:C:7:ALA:HB3	1:C:43:THR:CG2	2.43	0.45
1:C:138:ASP:HB2	2:D:105:MET:HE3	1.98	0.45
1:G:43:THR:HG22	1:G:105:THR:CG2	2.46	0.45
1:G:123:ARG:NH1	2:H:37:ASP:OD2	2.50	0.45
1:A:187:LEU:HB2	1:A:206:ILE:HD12	1.98	0.45
1:G:138:ASP:HB3	1:G:142:VAL:HG22	1.98	0.45
1:G:187:LEU:HB2	1:G:206:ILE:HD12	1.99	0.45
1:E:18:ILE:HG21	1:E:31:MET:HE2	1.99	0.45
2:D:61:ASP:OD1	3:D:127:PO4:O4	2.35	0.45
1:E:7:ALA:HB3	1:E:43:THR:CG2	2.44	0.44
1:E:133:ASN:HD21	1:E:148:ARG:NH2	2.15	0.44
1:G:18:ILE:HG21	1:G:29:ILE:HG21	1.97	0.44
1:G:212:THR:HG22	1:G:212:THR:O	2.18	0.43
1:G:46:PRO:O	1:G:47:LEU:HD23	2.17	0.43
1:A:123:ARG:HG2	2:B:110:TRP:CZ3	2.53	0.43
1:E:29:ILE:HD13	1:E:75:LEU:HB2	2.00	0.43
2:B:18:LEU:HB2	2:B:82:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LEU:HD21	1:G:162:VAL:CG1	2.49	0.43
1:E:25:LEU:HD21	1:E:52:TYR:HD2	1.84	0.43
1:G:206:ILE:HG23	1:G:217:VAL:HG12	2.01	0.43
1:C:187:LEU:HB3	1:C:206:ILE:HD12	2.01	0.43
1:E:125:MET:HE2	1:E:125:MET:HB2	1.95	0.42
2:H:51:ILE:HD13	2:H:71:ARG:HB2	2.01	0.42
1:C:217:VAL:HG12	1:C:224:ARG:HG2	2.01	0.42
1:E:67:VAL:HG11	1:E:75:LEU:HD22	2.00	0.42
1:E:115:VAL:HG13	1:E:141:ASN:CG	2.45	0.42
1:A:125:MET:HE2	1:A:125:MET:HB2	1.89	0.42
1:G:67:VAL:CG1	1:G:75:LEU:HD22	2.49	0.42
1:G:187:LEU:HB3	1:G:206:ILE:HD12	2.02	0.42
2:D:4:LEU:HD12	2:D:110:TRP:HA	2.00	0.42
2:D:34:MET:CE	2:D:95:CYS:SG	3.08	0.42
1:G:123:ARG:HG2	2:H:110:TRP:CZ3	2.55	0.42
2:B:99:VAL:HG21	2:B:109:TYR:HE1	1.85	0.41
1:C:112:ASN:ND2	1:C:167:ASN:HB2	2.36	0.41
1:E:43:THR:HA	1:E:105:THR:HG22	2.02	0.41
1:C:123:ARG:HG2	2:D:110:TRP:CZ3	2.56	0.41
1:E:105:THR:HA	1:E:145:LEU:O	2.20	0.41
1:E:182:GLU:O	1:E:186:VAL:HG23	2.20	0.41
2:B:63:VAL:HB	2:B:67:PHE:CD2	2.56	0.40
2:H:82:MET:HE1	2:H:116:VAL:HG21	2.03	0.40
1:A:145:LEU:HD22	1:A:155:LEU:HD13	2.03	0.40
1:E:118:LEU:HD21	1:E:162:VAL:CG1	2.48	0.40
3:D:127:PO4:P	2:H:71:ARG:HH21	2.44	0.40
2:D:99:VAL:HG21	2:D:109:TYR:HE2	1.87	0.40
2:F:18:LEU:HB2	2:F:82:MET:HE3	2.02	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	190/241 (79%)	180 (95%)	10 (5%)	0	100	100
1	C	189/241 (78%)	186 (98%)	3 (2%)	0	100	100
1	E	189/241 (78%)	182 (96%)	7 (4%)	0	100	100
1	G	191/241 (79%)	184 (96%)	7 (4%)	0	100	100
2	B	118/126 (94%)	118 (100%)	0	0	100	100
2	D	118/126 (94%)	118 (100%)	0	0	100	100
2	F	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
2	H	118/126 (94%)	116 (98%)	2 (2%)	0	100	100
All	All	1231/1468 (84%)	1201 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	174/205 (85%)	170 (98%)	4 (2%)	44	78
1	C	172/205 (84%)	169 (98%)	3 (2%)	53	83
1	E	172/205 (84%)	170 (99%)	2 (1%)	63	87
1	G	174/205 (85%)	172 (99%)	2 (1%)	65	87
2	B	97/103 (94%)	95 (98%)	2 (2%)	47	79
2	D	97/103 (94%)	96 (99%)	1 (1%)	68	88
2	F	97/103 (94%)	96 (99%)	1 (1%)	68	88
2	H	97/103 (94%)	96 (99%)	1 (1%)	68	88
All	All	1080/1232 (88%)	1064 (98%)	16 (2%)	57	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	113	VAL

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Mol	Chain	Res	Type
1	A	126	ILE
1	A	235	ASP
1	C	6	THR
1	C	113	VAL
1	C	126	ILE
1	E	72	ASN
1	E	211	ARG
1	G	39	VAL
1	G	206	ILE
2	B	12	VAL
2	B	35	ASP
2	D	12	VAL
2	F	12	VAL
2	H	33	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	177	ASN
1	E	63	GLN
1	E	112	ASN
1	E	133	ASN
1	G	112	ASN
2	B	58	ASN
2	B	81	GLN
2	B	83	ASN
2	B	98	ASN
2	D	1	GLN
2	D	81	GLN
2	F	3	GLN
2	F	81	GLN
2	F	98	ASN
2	H	81	GLN
2	H	98	ASN

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	PO4	H	127	-	4,4,4	0.99	0	6,6,6	0.75	0
3	PO4	E	238	-	4,4,4	0.96	0	6,6,6	1.01	0
3	PO4	G	238	-	4,4,4	0.92	0	6,6,6	0.69	0
3	PO4	C	238	-	4,4,4	0.95	0	6,6,6	0.59	0
3	PO4	A	238	-	4,4,4	1.08	0	6,6,6	0.67	0
3	PO4	F	127	-	4,4,4	0.90	0	6,6,6	0.74	0
3	PO4	B	127	-	4,4,4	1.05	0	6,6,6	0.68	0
3	PO4	D	127	-	4,4,4	1.01	0	6,6,6	0.32	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	127	PO4	1	0
3	D	127	PO4	2	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	198/241 (82%)	0.22	7 (3%) 47 38	37, 54, 70, 77	0
1	C	197/241 (81%)	0.21	10 (5%) 33 25	37, 53, 72, 77	0
1	E	197/241 (81%)	0.42	15 (7%) 20 14	37, 49, 77, 79	0
1	G	199/241 (82%)	0.51	16 (8%) 18 13	38, 52, 66, 68	0
2	B	120/126 (95%)	-0.36	1 (0%) 82 75	41, 45, 48, 50	0
2	D	120/126 (95%)	-0.18	1 (0%) 82 75	41, 45, 48, 50	0
2	F	120/126 (95%)	-0.20	1 (0%) 82 75	41, 45, 48, 50	0
2	H	120/126 (95%)	-0.30	1 (0%) 82 75	41, 45, 48, 50	0
All	All	1271/1468 (86%)	0.11	52 (4%) 41 33	37, 47, 67, 79	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	32	GLY	5.7
1	G	44	MET	4.4
1	E	220	ASP	4.0
1	G	6	THR	3.7
2	H	1	GLN	3.5
1	G	46	PRO	3.4
1	G	8	ASN	3.4
1	G	191	THR	3.3
1	E	221	PRO	3.2
1	G	45	THR	3.2
2	D	1	GLN	3.2
1	G	4	THR	3.1
1	E	219	GLY	3.1
1	E	224	ARG	3.1
1	A	235	ASP	3.1
1	G	5	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	210	GLU	3.0
1	A	100	GLY	2.9
2	F	1	GLN	2.8
1	C	30	ILE	2.7
1	G	42	ARG	2.7
1	G	47	LEU	2.6
1	E	218	SER	2.6
1	G	43	THR	2.6
1	C	210	GLU	2.6
1	C	31	MET	2.6
1	E	215	VAL	2.6
2	B	88	GLU	2.6
1	A	35	VAL	2.5
1	G	3	ALA	2.5
1	C	3	ALA	2.5
1	E	11	ASP	2.5
1	G	35	VAL	2.5
1	C	191	THR	2.4
1	E	208	ALA	2.4
1	C	28	THR	2.4
1	C	35	VAL	2.3
1	C	26	ASN	2.3
1	C	4	THR	2.3
1	G	99	ALA	2.3
1	E	172	VAL	2.3
1	A	3	ALA	2.3
1	E	235	ASP	2.2
1	A	219	GLY	2.1
1	E	4	THR	2.1
1	A	117	GLU	2.1
1	G	65	TYR	2.1
1	G	164	HIS	2.1
1	C	169	THR	2.0
1	E	222	ALA	2.0
1	E	180	ALA	2.0
1	E	217	VAL	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 [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($\text{\AA}^2$)	Q<0.9
4	CL	B	128	1/1	0.92	0.15	76,76,76,76	0
4	CL	D	128	1/1	0.93	0.12	69,69,69,69	0
3	PO4	H	127	5/5	0.95	0.15	57,58,58,59	0
4	CL	F	128	1/1	0.95	0.13	72,72,72,72	0
4	CL	H	128	1/1	0.95	0.11	72,72,72,72	0
3	PO4	G	238	5/5	0.96	0.17	55,55,56,57	0
3	PO4	B	127	5/5	0.96	0.17	58,58,59,60	0
3	PO4	F	127	5/5	0.96	0.21	56,57,57,58	0
3	PO4	E	238	5/5	0.96	0.10	55,55,57,58	0
3	PO4	C	238	5/5	0.97	0.14	50,51,51,52	0
3	PO4	A	238	5/5	0.97	0.13	59,59,60,61	0
3	PO4	D	127	5/5	0.97	0.15	46,46,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.